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A MODEL FOR PREDICTING THE GENERATION RATE AND DISTRIBUTION OF PRODUCTS OF COMBUSTION IN TWO-LAYER FIRE ENVIRONMENTS

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A MODEL FOR PREDICTING THE GENERATION RATE AND DISTRIBUTION OF PRODUCTS OF COMBUSTION IN TWO-LAYER FIRE ENVIRONMENTS

Leonard Y. Cooper

ABSTRACT

A model is developed for predicting the generation rates of oxygen, fuel, and any other products of combustion in rooms containing fires. The model is called the generalized global equivalence ratio model. It extends the steady state global equivalence ratio model established from steady-state data of several previous experimental studies. After describing the model in detail, a concise algorithm is outlined for implementing it in two-layer zone-type compartment fire model computer codes. With the algorithm in place, such codes could be used to simulate the distribution of combustion products in single or multi-room fire environments. In an example application, the model simulates the time-dependent environment, including that of steady-state, in some of the above-mentioned experimental studies. For arbitrary experimental conditions and under the assumption of complete stoichiometric combustion, solutions for concentrations of products of combustion are obtained and presented. The solutions are used to predict the time-to-extinguishment of a burning methane fuel source embedded in an initially ambient-atmosphere upper layer.

Keywords: **building fires; combustion; compartment fires; computer models; fire models; mathematical models; zone models.**

1. Introduction

The objective of this work is to develop a general model usable in two-layer zone-type compartment fire analyses, for predicting the generation rate and accumulation of combustion products throughout a multi-room facility. The model is called the Generalized Global Equivalence Ratio Model.

1.1 The Extended Upper-Layer in a Room Containing a Fire

Consider a multi-room compartment fire and assume an upper-layer/lower-layer zone-type of description of the environment in each of the rooms. As indicated in Figure 1, for the purpose of describing the combustion process, the fire and plume, which may protrude into the lower layer, is taken as part of the upper-layer zone. Also, the volume of any such protrusion is assumed to be negligible compared to the total volume of the room. Thus, as in [1], all combustion processes in any room with a fire are defined as occurring in the upper layer. The actual combustion process in this extended upper-layer zone will be modeled here as in a well-stirred reactor [2] with relatively rapid flowthrough and corresponding negligible residence time.

1.2. An Overview of the Generalized Global Equivalence Ratio Model

The purpose of this section is to provide a brief overview of the essential features of the Generalized Global Equivalence Ratio Model, the details of which are presented at length in the remainder of the paper.

The goal of the model is to estimate net rates of change of mass of combustion products k in the upper layer, $dP_{k,U}/dt$, for any room containing a fire in an arbitrary multi-room fire scenario. As depicted in Figure 2, the model has two components. These are the accumulator, which simulates the generally unsteady average environment of the upper layer, and the quasi-steady reactor, depicted in Figure 3, which simulates the actual combustion processes taking place there.

The material flowing into and out of the extended upper layer generally includes various amounts of the combustion products k associated with a fuel of interest and other inert flow components. The actual rates of inflow and outflow of product k, $\dot{P}_{k,FLOWIN}$ and $\dot{P}_{k,FLOWOUT}$, respectively, would be determined from compartment fire modeling considerations which are beyond the scope of this paper. These rates are assumed to be known.

As indicated in Figure 2, all of the flow into the layer is modeled as immediately "entering" the reactor where it participates in the reaction process. Also participating in the reaction process is a certain amount of bulk upper layer atmosphere. This is depicted in Figure 2 by the "feedback loop" flow which is also seen to "enter" the reactor. A critical feature of the overall model is that it always predicts reasonable results for the feedback mass flow rate, $\dot{m}_{FEEDBK}$. The algorithm for estimating $\dot{m}_{FEEDBK}$ is presented in Section 5.

ϕ, the global equivalence ratio, is a normalized ratio of the rates of fuel to oxygen entering the reactor. ϕ is defined and determined according to Eq. (7). Then the rate of generation of an arbitrary product k, $\dot{\omega}_k$, is found from Eq. (9), where the f_k functions for the fuel would be determined from steady state experiments of the type carried out in references [3]-[7]. Having obtained the $\dot{\omega}_k$, conservation of species leads to the desired result for $dP_{k,U}/dt$. This is obtained from Eqs. (1) and (4).

2. The Variables Computed in a Compartment Fire Model

At an instant of time of interest let $P_{k,U}$ and $P_{k,L}$ be the amount of product of combustion k in the upper and lower layers, respectively, of a room containing a fire. The products would include O_2, CO_2, H_2O, CO, unburned fuel, and any other products related to a particular fuel of interest. For the purpose of the present paper, these do not include inert components of the environment.

Together with hydrostatic pressure at some datum elevation in the room (e.g., at the floor), the elevation of the upper-layer/lower-layer interface, and the total mass in the upper and lower layers, it is convenient to use the $P_{k,U}$'s and $P_{k,L}$'s as basic solution variables in two-layer zone-type fire models. Also included in the basic set of solution variables are the pressures, interface elevations, masses, and $P_{k,U}$'s and $P_{k,L}$'s of all other rooms of the facility outside of rooms which actually contain a fire. While a $P_{k,U}$ and $P_{k,L}$ would correspond typically to the mass of product k, as is the case here, in a zone model formulation, it could also correspond to some other extensive property of the product, e.g., like total number of particles of product k or total number of particles of product k in a specified size range.

Variables derived from the basic solution variables are also required in analyses of the compartment fire environment. For example, the density of the layer can be calculated directly from the two solution variables: layer interface elevation (i.e., layer volume) and layer mass. Similarly, the mass concentrations of a product k in the upper and lower layer, $c_{k,U}$ and $c_{k,L}$, would be calculated from the values of $P_{k,U}$ and $P_{k,L}$ and the values of the upper- and lower-layer masses, m_U and m_L.

In a compartment fire model, generic equations for the solution variables $P_{k,U}$ and $P_{k,L}$ can be represented by the following basic equations of conservation of product k in the upper and lower layers [8]:

$$dP_{k,U}/dt = \dot{P}_{k,U} \tag{1}$$

$$dP_{k,L}/dt = \dot{P}_{k,L} \tag{2}$$

The right-hand-side terms, $\dot{P}_{k,U}$ and $\dot{P}_{k,L}$, represent the net rates of product of combustion k flowing to the upper and lower layer, respectively. These terms represent the sum of transfers of product k to the respective layers

from all plumes, jets, near-boundary flows, combustion zones, and other isolated or distributed sources considered and taken into account in any particular zone fire model. In this regard it is noteworthy that the number of types of flow and heat- and mass-transfer phenomena taken into account, and the detail and sophistication with which such phenomena are modeled are key distinguishing features between one zone fire model and another.

As mentioned above, it is assumed here that generation of products due to combustion processes occurs only in the extended upper layer of a room of fire origin. Thus, in the present formulation, $\dot{P}_{k,U}$, but not $\dot{P}_{k,L}$ can include generation-rate contributions due to combustion.

This paper presents a general model for including combustion processes in Eq. (1). It is applicable for general use in two-layer zone-type analyses of compartment fire scenarios. The model incorporates and extends the use of the steady state global equivalence ratio model which has been proposed and supported by steady-state data acquired previously in the two-layer experimental studies of references [3-7] and which has been discussed and analyzed in [1] in the context of a dynamic room fire environment.

3. Modeling the Combustion Process and the Unsteady Accumulation of Mass and Species in the Extended Upper Layer

3.1. Two Components of the Model

Depicted in Figure 2 is a model for flow, combustion, and mass- and combustion-product accumulation in fire scenarios occuring in the extended upper layer of Figure 1. As will be seen, the model can be used to simulate the reported steady state data of the various two-layer experiments of [3-7]. These are the data which were used to establish the steady state global equivalence ratio model. Also, as required to meet the objective of this work, the proposed model can be used in two-zone fire models to simulate the effects of combustion in unsteady, multi-room fire scenarios.

The model involves two interacting components, a reactor and an accumulator. These two components interact by way of a feedback loop which passes material, at a rate to be determined, from the generally unsteady, but spatially-uniform-property accumulator to the input stream of the quasi-steady reactor.

3.2. Modeling the Combustion Process - The Reactor

In the phenomena being simulated, combustion processes are confined to a well-mixed volume of the extended upper layer. Depending on a variety of factors, at one extreme this combustion zone can be insignificantly small and at the other can even dominate the entire layer. For example, in a Figure 1-type of fire scenario combustion is often confined to the lower portion of the relatively small-volume, turbulent fire plume. Sometimes a fire can grow to the point that combustion even extends beyond the fire-plume volume and into a significant portion of the relatively small-volume, turbulent ceiling jet, the latter being formed by impingement of the burning plume and the ceiling

surface. Under fuel rich conditions the combustion can fill most of the upper layer which itself can nearly fill the entire room.

The flow rates through the well-mixed combustion zone lead typically to characteristic residence times there which are small compared to the characteristic times of interest of the overall phenomena being modeled , but large compared to characteristic times of the combustion kinetics. This is the basis for modeling as quasi-steady the combustion processes.

All combustion processes are modeled by the reactor.

It is important to point out that the reactor component of the model has a strong conceptual aspect in the sense that it is not intended to correspond strictly to any physical subdivision of the extended upper layer. Thus, while the role of the reactor is to simulate all significant combustion processes, there is no accounting for physical boundaries that approximate the spatial limits of the combustion processes. For example, no material or material properties are associated with the "inside" of the reactor component, only material that enters and leaves it, and products of combustion that are generated by its action.

At least one aspect of the conceptual character of the reactor is highlighted in the model representation of Figure 2. As seen there, in the present model <u>all</u> flows entering the extended upper layer, pass through the reactor prior to being deposited in the accumulator. Yet, in the generic fire scenario depicted in Figure 1, it is clear that flows entering the upper layer from vents, e.g., from the doorway on the right side of the figure, do not enter directly a physical region of the extended upper layer that in any significant sense can be construed as the region wherein the significant combustion processes are taking place.

3.3. Modeling the Bulk of the Upper Layer - The Accumulator

As observed in room fires, it is reasonable to model the properties of the major portion of the extended upper-layer volume as spatially uniform. This is modeled by the accumulator.

Assuming that the instantaneous contents of the extended upper layer, of total mass, m_U, reside in the accumulator, the average concentrations of products there are

$$c_{k,U} = P_{k,U}/m_U \qquad (3)$$

This is indicated in Figure 2.

Throughout the rest of this work, the $P_{k,U}$ will correspond to the mass of product k in the upper layer of a space of fire origin. Therefore, $c_{k,U}$ will always represent the mass fraction of a product k.

The experimental data presented in references [3-7] were acquired under conditions of steady state. For this reason, an accumulator used in the modeling of those particular data would also be in a steady state. However, because the characteristic times for flows to pass through extended upper layers are typically relatively large, the properties of the accumulator in the model must be described generally as unsteady. In other words, the instantaneous rates of accumulation of products in the accumulator must be modeled as being generally non-zero and significant. The latter would be true even at times when the volume itself is relatively constant. As will be seen, such times of constant volume are exemplified by the transient upper layer environments in the experiments of references [3], [4], and [7], where these transients develop finally into the steady state conditions described by the actual data which are documented.

In difference to the reactor, the physical boundaries of the accumulator are well-defined, namely, they are well-approximated by the boundaries of the upper layer. Yet, as with the reactor, aspects of the accumulator component of the present model must also be regarded as conceptual. For example, as noted before in Figure 2, any vent flows that are deposited into the upper layer are modeled as entering the reactor (i.e., the combustion process) prior to actually flowing into and mixing with the bulk of the upper layer. Again this is clearly in difference to the physical picture depicted in Figure 1. The conceptual character of the accumulator is also related to the fact that it is assumed to interact directly with the reactor. Thus, it would appear that a model component (the accumulator) which interacts with a conceptual model component (the reactor) must itself be regarded as conceptual.

3.4. The Flow Exchanges Between the Reactor and the Accumulator; the Flow-Rate in the Feedback Loop

Depicted in Figure 2 are the components of flow to the extended upper layer and flow exchanges between the reactor and the accumulator.

In general, the net flow to the extended upper layer is made up of a series of unidirectional flow components, flow components <u>into</u> the layer and flow components <u>out of</u> the layer. As indicated in Figure 2, the sum of all flow components of product k <u>into</u> the layer is designated as $\dot{P}_{k,FLOWIN}$ and the sum of all flow components <u>out of</u> the layer is designated as $\dot{P}_{k,FLOWOUT}$. The $\dot{P}_{k,FLOWIN}$ are all modeled as flowing directly to the input of the reactor prior to entering the accumulator.

The combustion process in the reactor leads to mass-generation-rate source terms for the products k. These are designated by $\dot{\omega}_k$. Conservation of mass requires that the sum of all $\dot{\omega}_k$ is zero.

In view of the above, $\dot{P}_{k,U}$ on the right-hand-side of Eq. (1) is given by

$$\dot{P}_{k,U} = \dot{P}_{k,FLOWIN} - \dot{P}_{k,FLOWOUT} + \dot{\omega}_k \qquad (4)$$

All $\dot{P}_{k,FLOWOUT}$ are assumed to flow directly out of the extended upper layer from the accumulator, i.e., from the bulk of the upper layer. For example, in the depiction of the fire scenarios of Figure 1, the $\dot{P}_{k,FLOWOUT}$ have two components. One of these is the flow of the products in the stream which passes from the upper layer in the room of fire origin through the upper vent in the wall on the right side to the adjacent space. The other components of $\dot{P}_{k,FLOWOUT}$ are convected in the flow which is entrained into the relatively cool stream flowing into the fire room from the vent in the left wall. Because of its negative local buoyancy, this stream together with the entrained material from the upper layer flows downward and is deposited into the lower layer.

The $\dot{P}_{k,FLOWIN}$ are made up of the sums of all types of inflow components. These include contributions of products of combustion k entrained from the lower layer into the plume, supplied directly from the fuel source, and flowing into the layer from wall, ceiling, or floor vents. The sketch of the fire scenario of Figure 1 indicates one vent flow stream which contributes to the $\dot{P}_{k,FLOWIN}$. This is the stream flowing across the layer interface on the right and entering the upper layer. This stream is driven by the locally upward-buoyancy of the flow through the doorway on the right.

As indicated in Figure 2, the inflow to the reactor is made up of the net flow rates, $\dot{P}_{k,REACTIN}$ and their corresponding total mass flow rate, $\dot{m}_{REACTIN}$. The combustion processes in the reactor lead to the mass-generation-rate source terms, $\dot{\omega}_k$, which are depicted in the figures as separate inflows to the reactor (Figure 3) and to the overall extended upper layer (Figure 2).

For a given k, $\dot{P}_{k,REACTIN}$ has two components. One of these is $\dot{P}_{k,FLOWIN}$, which was discussed above. The other is $\dot{P}_{k,FEEDBK}$.

$$\dot{P}_{k,REACTIN} = \dot{P}_{k,FLOWIN} + \dot{P}_{k,FEEDBK} \tag{5}$$

$\dot{P}_{k,FEEDBK}$ is modeled as a product k flow rate introduced into the combustion process from the accumulator, i.e., from the bulk of the upper layer. This flow is represented by the feedback loop of Figure 2. The $\dot{P}_{k,FEEDBK}$ and their corresponding total mass flow rate, $\dot{m}_{FEEDBK}$, can be thought of as representing a portion of the flow entrained into the combustion zone from the bulk of the upper layer. By virtue of the fact that this portion of flow enters the reactor, it will always have an effect on the combustion process, i.e., it will lead to modification of the $\dot{\omega}_k$'s.

As will be seen, a critical task in modeling the combustion process involves the establishment of a uniformly valid means of estimating $\dot{m}_{FEEDBK}$. This must be consistent with (1) the steady state global equivalence ratio model, as established, for example, in [3-7] for certain limited, two-layer, steady-state combustion processes, and with (2) an arbitrary, unsteady, and fully-general two-layer zone-type description of a fire room environment.

As indicated in Figure 2, the output from the reactor, $\dot{P}_{k,REACTOUT}$, flows directly into the accumulator.

4. Previously Acquired Steady-State Data, the Global Equivalence Ratio, and the Reactor Combustion Process

4.1. The Inflow to the Reactor

The combustion within the reactor will be represented as having a direct correspondence with the combustion processes studied during steady state conditions in the experiments of [3-7]. Thus, in the present model, combustion will be simulated by relating reactor output to reactor input through direct application of the steady state global equivalence ratio model.

4.2. The Global Equivalence Ratio - A Model for the Reactor

Represent generally the reaction for a particular fuel of interest by

fuel + oxygen $\longrightarrow$ all reaction products, including excess oxygen and/or excess fuel and/or products of incomplete combustion

Also, assume that the chemical composition of the fuel volatiles are known. Then for continuous idealized stoichiometric combustion of the fuel it would be possible to calculate the ratio of rates of mass flow of fuel to oxygen.

$$r = (\dot{P}_{FUEL}/\dot{P}_{OXY})_{STOICH} \tag{6}$$

Here, idealized stoichiometric reactions of a C, H, O-types of fuels refer to reactions where fuel and oxygen are mixed in proportions that ideally would lead only to CO_2 and H_2O, with no excess fuel or oxygen.

It is assumed that r is known for a fuel of interest.

Consider the combustion of a fuel of interest. Define the global equivalence ratio, ϕ, as the instantaneous ratio of mass flow rates of fuel to oxygen supplied to the reactor, normalized by the idealized stoichiometric fuel-to-oxygen ratio

$$\phi \equiv (\dot{P}_{FUEL,REACTIN}/\dot{P}_{OXY,REACTIN})/r \tag{7}$$

This definition is equivalent to the ϕ-definitions of [3-7].

Since the combustion described by the reactor is assumed to be quasi-steady, i.e., the rates of accumulation of products of combustion there are taken to be zero, the rate at which a product k flows out of the reactor must satisfy

$$\dot{P}_{k,\mathrm{REACTOUT}} = \dot{P}_{k,\mathrm{REACTIN}} + \dot{\omega}_k \tag{8}$$

Note that for a product such as oxygen and fuel, which is consumed by the combustion process, $\dot{\omega}_k$ would be negative. Note also that inert flow components like N_2 would be associated with $\dot{\omega}_k \equiv 0$. As stated earlier, inert components are not the subject of the present paper.

As established in [3-7], the steady state global equivalence ratio model states that the mass generation rate of product k in the reactor per unit mass of fuel flowing into the reactor is a unique function of ϕ.

$$\dot{\omega}_k / \dot{P}_{\mathrm{FUEL,REACTIN}} = f_k(\phi) \tag{9}$$

Results reported in [7] indicate that the f_k's are also generally functions of temperature, the dependency becoming important only for upper layer temperatures which exceed 800-900 K. For now this dependence will be ignored.

Relative to the nomenclature of previous work, the f_k of Eq. (9) are identical to the "un-normalized yields" of [5] and [6].

In principle one would hope that Eq. (9) is applicable to many practical fuels and that a standard test method could be established to determine for a particular fuel the f_k functions for all product k's of interest. In developing and presenting the model it is assumed here that all such f_k functions for a fuel of interest have been so determined.

For the case of complete stoichiometric combustion, it can be shown from Eqs. (7)-(9) that

$$f_{\mathrm{OXY}}^{(\mathrm{STOICH})} = \begin{cases} -1/r & \text{if } 0 \le \phi \le 1 \\ -1/(r\phi) & \text{if } \phi > 1 \end{cases} \tag{10}$$

$$f_{\mathrm{FUEL}}^{(\mathrm{STOICH})} = \begin{cases} -1 & \text{if } 0 \le \phi \le 1 \\ -1/\phi & \text{if } \phi > 1 \end{cases} \tag{11}$$

Here, complete stoichiometric combustion means that: for fuel-lean inputs to the reactor, i.e., $0 \le \phi \le 1$, all input fuel is involved in an idealized stoichiometric reaction with the input oxygen; for fuel-rich inputs to the

reactor, i.e., $\phi > 1$, all input oxygen is involved in an idealized stoichiometric reaction with the input fuel.

If all of the $\dot{P}_{k,REACTIN}$ are known at a particular instant of time, then ϕ can be calculated from Eq. (7), $\dot{\omega}_k$ can then be calculated from Eq. (9), and all components of the reactor output can be determined finally from Eq. (8).

Assume that $\dot{m}_{REACTIN}$ and the $\dot{P}_{k,REACTIN}$ are known. Then using Eqs. (8) and (9), the mass concentrations of the reactor outflow, $c_{k,REACTOUT}$, can be calculated from

$$c_{k,REACTOUT} = [\dot{P}_{k,REACTIN} + \dot{P}_{FUEL,REACTIN} f_k(\phi)]/\dot{m}_{REACTIN} \tag{12}$$

Eq. (12) can also be expressed as

$$c_{k,REACTOUT} = c_{k,REACTIN}[1 + (\dot{P}_{FUEL,REACTIN}/\dot{P}_{k,REACTIN}) f_k(\phi)] \tag{13}$$

$$= c_{FUEL,REACTIN}[\dot{P}_{k,REACTIN}/\dot{P}_{FUEL,REACTIN} + f_k(\phi)] \tag{14}$$

$$= c_{OXY,REACTIN}[\dot{P}_{k,REACTIN}/\dot{P}_{OXY,REACTIN} + \phi f_k(\phi) r] \tag{15}$$

Eq. (8) and Eq. (14) or (15) with k → fuel leads to

$$c_{FUEL,REACTOUT} = c_{FUEL,REACTIN}[1 + f_{FUEL}(\phi)] \tag{16}$$

$$= c_{OXY,REACTIN} r\phi[1 + f_{FUEL}(\phi)] \tag{17}$$

Eq. (15) with k → oxygen leads to

$$c_{OXY,REACTOUT} = c_{OXY,REACTIN}[1 + \phi f_{OXY}(\phi) r] \tag{18}$$

For the case of complete stoichiometric combustion, Eqs. (10) and (11) in Eqs. (16) and (18), respectively, lead to

$$c_{FUEL,REACTOUT,STOICH} = \begin{cases} 0 & \text{if } 0 \le \phi \le 1 \\ (1 - 1/\phi) c_{FUEL,REACTIN} & \text{if } 1 < \phi \end{cases} \tag{19}$$

$$c_{OXY,REACTOUT,STOICH} = \begin{cases} (1 - \phi) c_{OXY,REACTIN} & \text{if } 0 \le \phi \le 1 \\ 0 & \text{if } 1 < \phi \end{cases} \tag{20}$$

4.3. A Requirement for Consistency Between the Reactor Model and Steady State Data Previously Acquired in Two-Layer Fire Experiments

The experiments of [3]-[7] involve burning of a fuel in a standard atmosphere somewhat below the upper layer. The experimental configuration used in [4] was similar to the one used in [5] and [6]. Both are depicted in Figure 4. As indicated in the figure, the work of [4] involved an inverted fire-gas collector with contents "pouring out" below its bottom edge (Figure 4b), while the work of [5] and [6] involved a similar inverted collector, but with side venting and with the layer contained fully within the vessel (Figure 4a). For the purpose of the present analysis, the two configurations do not involve any significant differences.

Also depicted in Figure 4c is the experimental configuration used in [3] and [7]. This is identical to that used in [4] except for the fact that here a steady flow of air was injected into the layer from many small holes near the top of the collector. This was done in a manner as to insure rapid mixing between the injected air and the the flow produced by the fire plume.

In all cases, data of [3]-[7] were reported for steady state conditions only. Indeed, it was for such steady state conditions that the data were used to establish and validate the steady state global equivalence ratio model presented in Section 4.2 and incorporated in the quasi-steady reactor portion of the present model.

The reactor model of Section 4.2 with the proposed feedback loop feature of Figure 2 is generally consistent with the [3]-[7] analyses of configuration 4-type steady state data if, at times of steady state, the feedback flow to the reactor is identically zero ($\dot{P}_{k,FEEDBK} = \dot{m}_{FEEDBK} = 0$). Consistency means that the generalized model provides predictions of product generation rates and product concentrations in the extended upper layer that are identical to predictions made by application of the steady state global equivalence ratio model. The stated consistency is clear from the sketch of Figure 2 where, with zero feedback to the reactor it is evident that the steady stream of combustion products at the reactor output would flow without further chemical reaction or alteration in concentration into and through a steady state accumulator ($\dot{P}_{k,REACTOUT} = \dot{P}_{k,FLOWOUT}$, $\dot{m}_{k,REACTOUT} = \dot{m}_{k,FLOWOUT}$, and $c_{k,REACTOUT} = c_{k,U}$).

Denote $c^{(SS)}_{FUEL,REACTOUT}$ and $c^{(SS)}_{OXY,REACTOUT}$ as the concentration of fuel and oxygen at the output of the reactor in the absence of any feedback. Then one criterion for consistency between the generalized equivalence ratio model and the steady state data of [3]-[7] is

> When $c_{FUEL,U} = c^{(SS)}_{FUEL,REACTOUT}$ and $c_{OXY,U} = c^{(SS)}_{OXY,REACTOUT}$ the generalized model should predict $\dot{P}_{k,FEEDBK} = \dot{m}_{FEEDBK} = 0$.

(21)

The proposed model satisfies the above criterion.

5. The Flow from the Accumulator to the Reactor - A Model for $\dot{m}_{FEEDBK}$

5.1 Considerations in the Establishment of the Feedback Flow Model

The feedback flow rate model is based on the following considerations:

a. The proposed generalized global equivalence ratio model must be completely consistent with the steady state global equivalence ratio model established through the steady state experimental studies of [3]-[7]. This consistency is guaranteed if:

   i. the product generation rates in the reactor satisfy the model equations outlined in Section 4.2; and

   ii. the feedback flow rate is zero identically under steady state conditions, and follows the criterion of (21).

b. When the feedback flow rate is nonzero, it is reasonable to assume that it is an explicit function of upper layer oxygen and fuel concentration. The present "first-order" model assumes a continuous, piecewise-linear functional relationship of form $\dot{m}_{FEEDBK} = \alpha_{FUEL}(c_{FUEL,U} - c^{(SS)}_{FUEL,REACTOUT}) + \alpha_{OXY}(c_{OXY,U} - c^{(SS)}_{OXY,REACTOUT})$ where $\dot{m}_{FEEDBK} \geq 0$, $\alpha_{FUEL} \geq 0$, and $\alpha_{OXY} \geq 0$.

c. It is reasonable to assume that for the following two classes of scenario and under generally unsteady conditions the feedback model should predict $\dot{m}_{FEEDBK} = 0$:

   i. concentration of fuel in the accumulator is zero, concentration of fuel in the reactor output in the absence of any feedback flow is non-zero, but, again in the absence of any feedback flow, the concentration of oxygen in the reactor output exceeds the concentration of oxygen in the accumulator; and

   ii. concentration of oxygen in the accumulator is zero, concentration of oxygen in the reactor output in the absence of any feedback flow is non-zero, but, again in the absence of any feedback flow, the concentration of fuel in the reactor output exceeds the concentration of fuel in the accumulator.

d. When the oxygen concentration in the accumulator is equal to some maximum achievable value and fuel concentration in the accumulator is zero, $\dot{m}_{FEEDBK}$ will be the minimum value that results in complete consumption of fuel in the reactor combustion process.

e. When the fuel concentration in the accumulator is equal to some maximum achievable value and oxygen concentration in the accumulator is zero, $\dot{m}_{FEEDBK}$ will be the minimum value that results in complete consumption of oxygen in the reactor combustion process.

The presentation in Section 5.2 will develop explicit general expressions, required in the feedback flow model, for the concentrations of products in the reactor output as a functions of concentrations of products in the reactor input, but in the absence of feedback flow. This will be done by invoking the above considerations of (a). In Section 5.3, these expressions will be related to the steady state concentration data acquired in the explicit experiments of references [3]-[7]. Following this, the complete model for $\dot{m}_{FEEDBK}$ satisfying the remaining considerations (b)-(d) will be presented in Section 5.4.

5.2. Definitions of ϕ_{FUEL} and ϕ_{OXY}; Concentrations in the Accumulator Under Steady State Conditions

Define $\phi^{(SS)}$ and $c^{(SS)}_{k,REACTOUT}$ as the values of ϕ and $c_{k,REACTOUT}$, respectively, during a virtual steady state condition defined by the current inflow rates, but with zero flow in the feedback loop, i.e., with $\dot{m}_{FEEDBK} = 0$.

$$\phi^{(SS)} \equiv (\dot{P}_{FUEL,FLOWIN}/\dot{P}_{OXY,FLOWIN})/r \tag{22}$$

(Note that $\phi^{(SS)}$ is identical to the ϕ_ℓ of [3], [4], and [7] and to ϕ of [5] and [6].) Then Eqs. (12), (16), and (18) lead to

$$c^{(SS)}_{k,REACTOUT} = [\dot{P}_{k,FLOWIN} + \dot{P}_{FUEL,FLOWIN} f_k(\phi^{(SS)})]/\dot{m}_{FLOWIN} \tag{23}$$

$$c^{(SS)}_{FUEL,REACTOUT} = c_{FUEL,FLOWIN}[1 + f_{FUEL}(\phi^{(SS)})] \tag{24}$$

$$c^{(SS)}_{OXY,REACTOUT} = c_{OXY,FLOWIN}[1 + \phi^{(SS)} f_{OXY}(\phi^{(SS)})r] \tag{25}$$

For a fuel of interest, define ϕ_{FUEL} as the maximum value of ϕ which leads to complete consumption of fuel, i.e., which leads to $\dot{P}_{FUEL,REACTOUT} = 0$. Using Eq. (8) and (9) with k → fuel, it can be shown that ϕ_{FUEL} satisfies

$$\phi_{FUEL} = \text{maximum root of } f_{FUEL}(\phi_{FUEL}) + 1 = 0 \tag{26}$$

Define similarly ϕ_{OXY} as the minimum value of ϕ which leads to complete consumption of oxygen, i.e., which leads to $\dot{P}_{OXY,REACTOUT} = 0$.

$$\phi_{OXY} = \text{minimum root of } \phi_{OXY} f_{OXY}(\phi_{OXY})r + 1 = 0 \tag{27}$$

For a combustion system involving complete stoichiometric combustion, $\phi_{FUEL} = \phi_{OXY} = 1$ and, using Eqs. (10) and (11), Eqs. (24) and (25) become

$$c^{(SS)}_{FUEL,REACTOUT,STOICH} = \begin{cases} 0 \text{ if } 0 \le \phi^{(SS)} \le 1 \\ (1 - 1/\phi^{(SS)})c_{FUEL,FLOWIN} \text{ if } 1 < \phi^{(SS)} \end{cases} \quad (28)$$

$$c^{(SS)}_{OXY,REACTOUT,STOICH} = \begin{cases} (1 - \phi^{(SS)})c_{OXY,FLOWIN} \text{ if } 0 \le \phi^{(SS)} \le 1 \\ 0 \quad \text{if } 1 < \phi^{(SS)} \end{cases} \quad (29)$$

For real systems, $0 < \phi_{FUEL} < 1 < \phi_{OXY}$.

5.3 Steady State Concentrations and the Experiments of [3]-[7]

Before presenting the model for $\dot{m}_{FEEDBK}$, the results of the last section will first be related to steady state data of the experiments of [3]-[7]. Each of those references present data which are directly related to the mass fraction concentrations of products in the upper layer. Because of the steady state condition, these concentrations are predicted by the model to be the $c^{(SS)}_{k,REACTOUT}$ of Eqs. (23)-(25). In the experiments, since flow to the upper layer is only from a "pure" fuel source and from air of a standard atmosphere, it is reasonable to assume the $\dot{P}_{k,FLOWIN}$ to be negligible for all (non-inert) products k other than fuel and oxygen. Therefore, Eq. (23) can be written as

$$c^{(SS)}_{k,REACTOUT} = c_{FUEL,FLOWIN} f_k(\phi^{(SS)}) \text{ for k other than fuel or oxygen} \quad (30)$$

Also, using Eq. (22) and the fact that the mass fraction of oxygen in air is 0.232 it can be shown that

$$c_{FUEL,FLOWIN} = 0.232\phi^{(SS)}r/(1 + 0.232\phi^{(SS)}r) \quad (31)$$

$$c_{OXY,FLOWIN} = 0.232/(1 + 0.232\phi^{(SS)}r) \quad (32)$$

Finally, Eqs. (31) and (32) in Eqs. (24), (25), and (30) leads to

For experiments of references [3]-[7]:

$$c^{(SS)}_{FUEL,REACTOUT} = 0.232\phi^{(SS)}r[1 + f_{FUEL}(\phi^{(SS)})]/(1 + 0.232\phi^{(SS)}r) \quad (33)$$

$$c^{(SS)}_{OXY,REACTOUT} = 0.232[1 + \phi^{(SS)}f_{OXY}(\phi^{(SS)})r]/(1 + 0.232\phi^{(SS)}r) \quad (34)$$

$$c^{(SS)}_{k,REACTOUT} = 0.232\phi^{(SS)}f_k(\phi^{(SS)})r/(1 + 0.232\phi^{(SS)}r) \text{ for k other than fuel or oxygen} \quad (35)$$

It can be shown that fuel and oxygen concentrations for complete stoichiometric combustion, as given in Eqs. (19) and (20), respectively, are properly recovered when $f_{OXY}^{(STOICH)}$ of Eq. (11) and $f_{FUEL}^{(STOICH)}$ of Eq. (10) are used in Eqs. (33) and (34), respectively.

The results of Eqs. (33)-(35) reafirm the consistency of the generalized global equivalency ratio model proposed here and the steady state global equivalence ratio model as established in the experiments of [3]-[7]. Thus, for a given fuel, i.e., for a fixed value of $(\dot{P}_{FUEL}/\dot{P}_{OXY})_{STOICH}$, the model predicts that under steady state conditions the concentrations of any product of combustion k in the bulk of the upper layer is a function only of $\phi^{(SS)}$ and $f_k(\phi^{(SS)})$. Given a reference [3]-[7]-type of experiment which uses a fuel with known r, it is therefore clear that steady state data in the form of a plot of $c_{k,REACTOUT}^{(SS)}$ as a function of $\phi^{(SS)}$ can be used to obtain any of the $f_k(\phi)$.

To illustrate this, consider data presented in [7] which were obtained from experiments with natural gas. Assume the fuel to be pure methane, CH_4. Then the stoichiometric reaction is $CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$, and it follows that

$$r = (\dot{P}_{CH4}/\dot{P}_{OXY})_{STOICH} = 16/64 = 1/4 \tag{36}$$

Using Eq. (36) in Eqs. (33)-(35) leads to

For the experiments of references [3]-[7] using methane as the fuel:

$$c_{CH4,REACTOUT}^{(SS)} = (0.232/4)\phi^{(SS)}[1 + f_{CH4}(\phi^{(SS)})]/[1 + (0.232/4)\phi^{(SS)}] \tag{37}$$

$$c_{OXY,REACTOUT}^{(SS)} = 0.232[1 + (1/4)\phi^{(SS)} f_{OXY}(\phi^{(SS)})]/[1 + (0.232/4)\phi^{(SS)}] \tag{38}$$

$$c_{k,REACTOUT}^{(SS)} = (0.232/4)\phi^{(SS)} f_k(\phi^{(SS)})/[1 + (0.232/4)\phi^{(SS)}] \quad \text{for k other than fuel or oxygen} \tag{39}$$

The right hand sides of Eqs. (37)-(39) are used to provide additional labels on the data plots, presented in Figures 1-4 of [7] and reproduced here in Figures 5-8. These plots are for the steady state upper layer mass fractions of O_2, CH_4, CO, and H_2, respectively, i.e., for the experimentally determined values of $c_{k,REACTOUT}^{(SS)}(\phi^{(SS)})$. In Figures 5-8, it should be noted that the steady state data of Toner were acquired in experiments where temperatures were higher than 900 K [7]. As stated below Eq. (9), the present model would not be expected to provide accurate predictions of these data. The Toner data in the plots of Figures 5-8 should be ignored from present consideration.

Note that for methane, Eq. (26) with Figure 5 and Eq. (27) with Figure 6 result in $\phi_{CH4} \approx 0.7$ and $\phi_{OXY} \approx 3.0$, respectively.

Consistent with the steady state global equivalence ratio model, the relevant data of Figures 5-8 are all well-correlated, i.e., the measured $c_{k,REACTOUT}^{(SS)}(\phi^{(SS)})$ data can be approximated by curve-fit functions $c_{k,REACTOUT}^{(SS,FIT)}(\phi^{(SS)})$. Using Eqs. (37)-(39), such curve fit functions could then be used to calculate the f_k's for methane from:

For methane:

$$f_{CH4}(\phi) = c_{CH4,REACTOUT}^{(SS,FIT)}(\phi)[1 + (4/0.232)/\phi] - 1 \qquad (37')$$

$$f_{OXY}(\phi) = c_{OXY,REACTOUT}^{(SS,FIT)}(\phi) + (4/\phi)[c_{OXY,REACTOUT}^{(SS,FIT)}(\phi)/0.232 - 1] \qquad (38')$$

$$f_k(\phi) = c_{k,REACTOUT}^{(SS,FIT)}(\phi)[1 + (4/0.232)/\phi] \text{ for k other than fuel and oxygen} \qquad (39')$$

Note that in Eqs. (37')-(39') the apparent singularities at $\phi = 0$ can be removed when one takes note of the fact that $c_{OXY,REACTOUT}^{(SS,FIT)}(0) = 0.232$ and $c_{k,REACTOUT}^{(SS,FIT)}(0) = 0$ for fuel and, as assumed here, for all other products in the experiments under consideration.

5.4 The Model for $\dot{m}_{FEEDBK}$

Presented in this section is a model for $\dot{m}_{FEEDBK}$ which satisfies all considerations outlined in Section 5.1. Three possible cases are considered: Case 1: $c_{OXY,U} \geq 0$, $c_{FUEL,U} = 0$; Case 2: $c_{OXY,U} \geq 0$, $c_{FUEL,U} \geq 0$; and Case 3: $c_{OXY,U} = 0$, $c_{FUEL,U} \geq 0$.

Case 1: $c_{OXY,U} \geq 0$, $c_{FUEL,U} = 0$

Here it is assumed that $\dot{m}_{FEEDBK} \equiv \dot{m}_{FEEDBK,1}$ (where the subscript 1 is associated with present Case 1) is proportional to $c_{OXY,U} - c_{OXY,REACTOUT}^{(SS)}$, if $c_{OXY,U} - c_{OXY,REACTOUT}^{(SS)} \geq 0$, and that $\dot{m}_{FEEDBK}$ is zero if $c_{OXY,U} - c_{OXY,REACTOUT}^{(SS)} < 0$. Thus, provided $\phi^{(SS)} \geq \phi_{FUEL}$, it is assumed that a relatively high concentration of oxygen in the bulk of the upper layer (i.e., compared to the concentration of oxygen in the virtual steady state) will enhance combustion in the reactor leading to $c_{OXY,REACTOUT} > c_{OXY,REACTOUT}^{(SS)}$, while a relatively low concentration of oxygen in the layer will not generally affect the combustion at all. Note that in the latter situation, where feedback is zero, the $c_{OXY,U}$ of the layer will tend to be increased by the relatively rich oxygen concentration of the reactor output, $c_{OXY,REACTOUT}^{(SS)}$, but that this will occur by a simple mixing process. The above assumptions are expressed as

$$\dot{m}_{FEEDBK,1} = \begin{cases} \dot{m}^{(1)}_{FEEDBK}(c_{OXY,U} - c^{(SS)}_{OXY,REACTOUT})/ \\ \qquad (c^{(MAX)}_{OXY,U} - c^{(SS)}_{OXY,REACTOUT}) \\ \qquad\qquad \text{if } c_{OXY,U} - c^{(SS)}_{OXY,REACTOUT} \geq 0 \\ 0 \text{ if } (c_{OXY,U} - c^{(SS)}_{OXY,REACTOUT}) < 0 \end{cases} \tag{40}$$

where $c^{(MAX)}_{OXY,U}$ is the maximum possible value of $c_{OXY,U}$, taken to be 0.232, and where $\dot{m}^{(1)}_{FEEDBK}$, the characteristic value of $\dot{m}_{FEEDBK,1}$, is taken to be the minimum feedback mass flow-rate from a $c^{(MAX)}_{OXY,U}$ upper layer environment to the reactor input stream which, together with the $\dot{P}_{OXY,FLOWIN}$ oxygen flow rate, would consume completely the $\dot{P}_{FUEL,FLOWIN}$ fuel flow rate. Thus, for $\phi^{(SS)} \leq \phi_{FUEL}$ (no fuel in the reactor output stream under zero feedback conditions), $\dot{m}^{(1)}_{FEEDBK} = 0$, while for $\phi^{(SS)} \geq \phi_{FUEL}$, the combined flow rate of oxygen, $\dot{m}^{(1)}_{FEEDBK} c^{(MAX)}_{OXY,U} + \dot{P}_{OXY,FLOWIN}$, and flow rate of fuel, $\dot{P}_{FUEL,FLOWIN}$, to the reactor input leads, by definition, to $\phi = \phi_{FUEL}$, i.e.,

$$\phi_{FUEL} = [\dot{P}_{FUEL,FLOWIN}/(\dot{m}^{(1)}_{FEEDBK} c^{(MAX)}_{OXY,U} + \dot{P}_{OXY,FLOWIN})]/r \tag{41}$$

Solving Eq. (41) for $\dot{m}^{(1)}_{FEEDBK}$

$$\dot{m}^{(1)}_{FEEDBK} = \begin{cases} 0 \text{ if } \phi^{(SS)}/\phi_{FUEL} \leq 1 \\ (1 - \phi_{FUEL}/\phi^{(SS)})\dot{P}_{FUEL,FLOWIN}/(c^{(MAX)}_{OXY,U}\phi_{FUEL} r) \\ \qquad\qquad \text{if } \phi^{(SS)}/\phi_{FUEL} > 1 \end{cases} \tag{42}$$

For stoichiometric reactions Eqs. (40) and (42) become

$$\dot{m}_{FEEDBK,1,STOICH} = \begin{cases} 0 \text{ if } 0 \leq \phi^{(SS)} \leq 1 \\ (1 - 1/\phi^{(SS)})(c_{OXY,U}/c^{(MAX)}_{OXY,U})\dot{P}_{FUEL,FLOWIN}/(c^{(MAX)}_{OXY,U} r) \\ \qquad\qquad \text{if } 1 < \phi^{(SS)} \end{cases} \tag{43}$$

An example of a Case-1 fire scenario is one where the upper layer is established with an environment of substantially normal atmospheric oxygen concentration and negligible fuel, i.e., $c_{OXY,U} \approx 0.232$ and $c_{FUEL,U} \approx 0$. For such fire scenarios, $\phi^{(SS)}$ can range from values close to 0, e.g., relatively large entrainment of air (oxygen) into the portion of the plume below the

layer interface, to arbitrarily large values, e.g., no oxygen enters the upper layer from below the layer interface. The latter situation would correspond to a case where the fuel source is actually submerged in the upper layer, e.g. as in the configuration in Figure 4b.

An analysis of this example will be presented below in Section 7.

It is convenient to consider Case 3 before Case 2.

Case 3: $c_{OXY,U} = 0$, $c_{FUEL,U} \geq 0$

Here it is assumed that $\dot{m}_{FEEDBK} \equiv \dot{m}_{FEEDBK,3}$ (where the subscript 3 is associated with the present Case 3) is proportional to $c_{FUEL,U} - c^{(SS)}_{FUELREACTOUT}$ if $c_{FUEL,U} - c^{(SS)}_{FUELREACTOUT} \geq 0$, and that $\dot{m}_{FEEDBK}$ is zero if $c_{FUEL,U} - c^{(SS)}_{FUELREACTOUT} < 0$. Thus, provided $\phi^{(SS)} < \phi_{OXY}$, it is assumed that a relatively high concentration of fuel in the bulk of the upper layer (i.e., compared to the concentration of fuel in the virtual steady state) will enhance combustion in the reactor leading to $c_{FUEL,REACTOUT} > c^{(SS)}_{FUELREACTOUT}$, while a relatively low concentration of fuel in the layer will not generally affect the combustion at all. Note that in the latter situation, where feedback is zero, the low $c_{FUEL,U}$ of the layer will tend to be increased by the relatively rich fuel concentration of the reactor output, $c^{(SS)}_{OXY,REACTOUT}$, but that this will occur by a simple mixing process. The above assumptions are expressed as

$$\dot{m}_{FEEDBK,3} = \begin{cases} \dot{m}^{(3)}_{FEEDBK}(c_{FUEL,U} - c^{(SS)}_{FUEL,REACTOUT})/ \\ \qquad (c^{(MAX)}_{FUEL,U} - c^{(SS)}_{FUEL,REACTOUT}) \\ \qquad \text{if } c_{FUEL,U} - c^{(SS)}_{FUELREACTOUT} \geq 0 \\ 0 \text{ if } c_{FUEL,U} - c^{(SS)}_{FUELREACTOUT} < 0 \end{cases} \tag{44}$$

where $c^{(MAX)}_{FUEL,U}$ is the maximum possible value of $c_{FUEL,U}$, taken to be 1, and where $\dot{m}^{(3)}_{FEEDBK}$, the characteristic value of $\dot{m}_{FEEDBK,3}$, is taken to be the minimum feedback mass flow rate from a $c^{(MAX)}_{FUEL,U}$ upper layer environment to the reactor input stream which, together with the $\dot{P}_{FUEL,FLOWIN}$ fuel flow rate, would consume completely the $\dot{P}_{OXY,FLOWIN}$ oxygen flow rate. Thus, for $\phi^{(SS)} \geq \phi_{OXY}$ (no oxygen in the reactor output stream under zero feedback conditions), $\dot{m}^{(3)}_{FEEDBK} = 0$, while for $\phi^{(SS)} < \phi_{OXY}$, the combined flow-rate of fuel, $\dot{m}^{(3)}_{FEEDBK} c^{(MAX)}_{FUEL,U} + \dot{P}_{FUEL,FLOWIN}$, and flow-rate of oxygen, $\dot{P}_{OXY,FLOWIN}$, to the reactor input leads, by definition, to $\phi = \phi_{OXY}$, i.e.,

$$\phi_{OXY} = [(\dot{P}_{FUEL,FLOWIN} + \dot{m}^{(3)}_{FEEDBK} c^{(MAX)}_{FUEL,U})/\dot{P}_{OXY,FLOWIN}]/r \tag{45}$$

Solving for $\dot{m}^{(3)}_{FEEDBK}$

$$\dot{m}^{(3)}_{FEEDBK} = \begin{cases} 0 \text{ if } \phi_{OXY}/\phi^{(SS)} \leq 1 \\ (1 - \phi^{(SS)}/\phi_{OXY})\dot{P}_{OXY,FLOWIN}\phi_{OXY}/(c^{(MAX)}_{FUEL,U}r) \text{ if } \phi_{OXY}/\phi^{(SS)} > 1 \end{cases} \tag{46}$$

For complete stoichiometric reactions Eqs. (44) and (46) become

$$\dot{m}_{FEEDBK,3,STOICH} = \begin{cases} (1 - \phi^{(SS)})(c_{FUEL,U}/c^{(MAX)}_{FUEL,U})\dot{P}_{OXY,FLOWIN}/(c^{(MAX)}_{FUEL,U}r) \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{if } 0 \leq \phi^{(SS)} \leq 1 \\ 0 \text{ if } 1 < \phi^{(SS)} \end{cases} \tag{47}$$

An example of a Case-3 fire scenario is one where the upper layer is established with an environment of pure fuel, i.e., $c_{OXY,U} \approx 0$ and $c_{FUEL,U} \approx 1$. Then, if $\phi^{(SS)} < \phi_{OXY}$ and if a burning fuel source is located below the layer interface, some oxygen introduced into the upper layer would react with the upper-layer fuel. Note that here a $\phi^{(SS)} = 0$ condition can be established if a source of oxygen (and an initial ignitor) is submerged completely in the upper layer.

The latter example involves an idealized scenario in that $c_{FUEL,U} \approx 1$ would not occur in a typical situation where the room containing the fire has a non-zero lower layer with a non-zero concentration of oxygen. This is the case since, as the fuel concentration in the upper layer increased from zero, ignition and burning at the layer interface and in the layer itself would occur at a characteristic fuel concentration significantly less than 1 [8]. Ignition criteria for initiation of such layer burning would be determined from the concentrations of oxygen and combustible species in the upper and lower layers.

Case 2: $c_{OXY,U} \geq 0$, $c_{FUEL,U} \geq 0$

For this case it is assumed that $\dot{m}_{FEEDBK} \equiv \dot{m}_{FEEDBK,2}$ is the maximum of $\dot{m}_{FEEDBK,1}$ and $\dot{m}_{FEEDBK,3}$.

$$\dot{m}_{FEEDBK,2} = \max(\dot{m}_{FEEDBK,1}, \dot{m}_{FEEDBK,3}) \tag{48}$$

All Cases:

Noting that Eq. (48) reduces to Eq. (40) or (43) if $c_{FUEL,U} = 0$ and that Eq. (48) reduces to Eq. (44) or (47) if $c_{OXY,U} = 0$, it is evident that Eq. (48) predicts $\dot{m}_{FEEDBK}$ uniformly for every possible fire scenario, i.e., for all cases 1, 2, and 3. It is therefore concluded that in general

$$\dot{m}_{FEEDBK} = \max(\dot{m}_{FEEDBK,1}, \dot{m}_{FEEDBK,3}) \tag{49}$$

where $\dot{m}_{FEEDBK,1}$ and $\dot{m}_{FEEDBK,3}$ are computed from Eqs. (40) or (43) and (44) or (47), respectively.

6. The Generalized Global Equivalence Ratio Model - An Algorithm for Invoking Conservation of Products of Combustion in the Upper Layer of a Room Containing a Fire

With the results of the last section it is now possible to construct an algorithm which uses the generalized global equivalence ratio model to invoke conservation of products of combustion, Eq. (1), in the upper layer of a room of fire origin.

Consider the simulation of a fire scenario involving a multi-room facility. Assume that the values of all solution variables and derived variables for all rooms are known at an instant of time during the simulation. This includes the concentrations of all products of combustion in all of the layers. It is assumed that the components of all mass inflows and outflows to each upper and lower layer in the facility have been computed according to the modeling details of a particular compartment fire model of interest. Also computed are the rates at which the products of combustion are convected to the layers by these inflows and outflows. This would be obtained from the known concentrations and flow rates. The product flow rates together with the instantaneous rate at which products are generated in the (extended) upper layers of rooms with fires make up the contributions, indicated in Eq. (4), to the right side of Eqs. (1) and (2). For all layers without combustion, i.e., where all $\dot{\omega}_k = 0$, Eqs. (1) and (2) is available for integration to the next time-step without any further consideration.

Consider an extended upper layer which includes combustion. It is assumed for the particular burning fuel that r, $f_{FUEL}(\phi)$, $f_{OXY}(\phi)$ and the $f_k(\phi)$ for the other product k's of interest have been obtained. As with all other layers, the $\dot{P}_{k,FLOWIN}$ and $\dot{P}_{k,FLOWOUT}$ of Eq. (4) are assumed to be available. Here, completion of the right side of Eq. (1) and integration to the next time step requires an estimate for the generally unknown $\dot{\omega}_k$'s. The following is the proposed procedure for obtaining such an estimate:

a. Determine $\phi^{(SS)}$ from Eq. (22).

b. Determine $\dot{m}_{FEEDBK}$ from Eq. (49).

c. From the known values of $c_{k,U}$, determine the $\dot{P}_{k,FEEDBK} = \dot{m}_{FEEDBK} c_{k,U}$ and use these in Eq. (5) with the known values of $\dot{P}_{k,FLOWIN}$ to determine the $\dot{P}_{k,REACTIN}$.

d. With the now-known values of $\dot{P}_{FUEL,REACTIN}$ and $\dot{P}_{OXY,REACTIN}$, determine ϕ from Eq. (7) and then the $\dot{\omega}_k$'s from Eq. (9).

7. Predicting $c_{k,U}$ in the Experiments of [3], [4], and [7] From the Initial Condition to Steady State - An Example Application of the Generalized Global Equivalence Ratio Model

7.1 The Initial Value Problem for the $c_{k,U}$

Use of the generalized global equivalence ratio model will now be illustrated. The model will be used to formulate generally, and solve under special conditions, the history of the $c_{k,U}$ of [3], [4], and [7], from the onset of the experiments to late times when steady state conditions are approached.

The configuration for the experiments of [3], [4], and [7] was such that the volume of the layer throughout most of a run was always approximately constant and equal to the volume of the collector. This is embodied in the first of the following assumptions:

a. the upper-layer volume, V, is fixed at the volume of the collector and is initially pure air, i.e., no non-inert components except for oxygen with a mass fraction of 0.232.

b. flow rates of fuel from the fuel source and oxygen from lower-layer entrainment are specified, and inflows of all other products of combustion from lower-layer entrainment are negligible;

c. the upper layer can be reasonably modeled as an ideal gas where properties are identical to those of air and where the absolute pressure is well-approximated by p_{ATM}, a characteristic pressure of the ambient;

d. the temperature history, $T_U(t)$, of the upper layer is known, and $T(0) = T_{AMB}$, the temperature of the laboratory; and

e. for the fuel being burned, the functions $f_k(\phi)$ for all products of interest are known.

Using Eqs. (1) and (3) leads to

$$dP_{k,U}/dt = d(m_U c_{k,U})/dt = m_U dc_{k,U}/dt + c_{k,U} dm_U/dt \quad (50)$$

$$m_U dc_{k,U}/dt + c_{k,U} dm_U/dt = \dot{P}_{k,REACTOUT} - \dot{P}_{k,FEEDBK} - \dot{P}_{k,FLOWOUT} \quad (51)$$

where the terms on the right of Eq. (51) are

$$\dot{P}_{k,REACTOUT} = (\dot{m}_{FEEDBK} + \dot{m}_{FLOWIN}) c_{k,REACTOUT} \quad (52)$$

$$\dot{P}_{k,FEEDBK} = \dot{m}_{FEEDBK} c_{k,U} \quad (53)$$

$$\dot{P}_{k,FLOWOUT} = \dot{m}_{FLOWOUT} c_{k,U} \quad (54)$$

Also, conservation of mass requires

$$dm_U/dt = \dot{m}_{FLOWIN} - \dot{m}_{FLOWOUT} \quad (55)$$

Using Eqs. (52)-(55) in Eq. (51) leads to

$$m_U dc_{k,U}/dt = (c_{k,REACTOUT} - c_{k,U})(\dot{m}_{FLOWIN} + \dot{m}_{FEEDBK}) \quad (56)$$

7.1.1 The Problem for $c_{FUEL,U}$ and $c_{OXY,U}$

For k → fuel or oxygen, it can be shown from Eqs. (16) and (18) that Eq. (56) can be written as

$$m_U dc_{FUEL,U}/dt = c_{FUEL,U}\dot{m}_{FEEDBK} f_{FUEL}(\phi) - c_{FUEL,U}\dot{m}_{FLOWIN} + \dot{P}_{FUEL,FLOWIN}[1 + f_{FUEL}(\phi)] \quad (57)$$

$$m_U dc_{OXY,U}/dt = c_{OXY,U}\dot{m}_{FEEDBK}\phi f_{OXY}(\phi) r - c_{OXY,U}\dot{m}_{FLOWIN} + \dot{P}_{OXY,FLOWIN}[1 + \phi f_{OXY}(\phi) r] \quad (58)$$

where

$$\phi = [(\dot{P}_{FUEL,FLOWIN} + c_{FUEL,U}\dot{m}_{FEEDBK})/(\dot{P}_{OXY,FLOWIN} + c_{OXY,U}\dot{m}_{FEEDBK})]/r \quad (59)$$

$$\dot{m}_{FEEDBK} = \dot{m}_{FEEDBK}(\text{inflow conditions}, c_{FUEL,U}, c_{OXY,U}) \quad (60)$$

and where $\dot{m}_{FEEDBK}$ of Eq. (60) is determined from Eq. (49).

The equation of state for the upper layer leads to

$$m_U = V\rho_U = Vp_{AMB}/(RT_U) \quad (61)$$

where ρ_U is the density of the upper layer and R is the gas constant for air. Based on assumption d. above Eq. (50), available data on $T_U(t)$ together with Eq. (61) yield an estimate for $m_U(t)$ throughout the entire experiment.

Eqs. (57) and (58) are the differential equations for predicting $c_{FUEL,U}$ and $c_{OXY,U}$ from t = 0 to steady state. To solve these, the right hand sides would be determined from Eqs. (59) and (60) and from the assumed known functions $f_{FUEL}(\phi)$ and $f_{OXY}(\phi)$ for the fuel used in the experiment.

The equations must be solved subject to the initial conditions

$$c_{FUEL,U}(t = 0) = 0 \quad (62)$$

$$c_{OXY,U}(t = 0) = c_{OXY,U}^{(MAX)} = 0.232 \quad (63)$$

7.1.2 The Problem For $c_{k,U}$, For k Other Than Fuel or Oxygen

Consistent with the discussion above Eq. (30), for the experiments of [3], [4], and [7] it is reasonable to assume

$$\dot{P}_{k,FLOWIN} = 0 \quad \text{for k other than fuel or oxygen} \quad (64)$$

Using Eqs. (64), (14), and (15) in Eq. (56) it can be shown that the initial value problems for the $c_{k,U}$ can be written as

for k other than fuel or oxygen:

$$m_U dc_{k,U}/dt + c_{k,U}\dot{m}_{FLOWIN} = (c_{FUEL,U}\dot{m}_{FEEDBK} + \dot{P}_{FUEL,FLOWIN})f_k(\phi) \quad (65)$$

$$= (c_{OXY,U}\dot{m}_{FEEDBK} + \dot{P}_{OXY,FLOWIN})\phi f_k(\phi)r \quad (66)$$

$$= \lambda_k(t) \quad (67)$$

$$c_{k,U}(t = 0) = 0 \quad (68)$$

Once the solutions of Eqs. (57)-(63) for $c_{FUEL,U}$ and $c_{OXY,U}$ have been obtained, the $\lambda_k(t)$ of Eq. (67) are known. $c_{k,U}$, for other products of interest would then be obtained from solutions of Eqs. (67) and (68).

7.2 Solution For the $c_{k,U}$ Under the Assumption of Complete Stoichiometric Combustion

7.2.1 The Functions $f_k(\phi)$ For k Other Than Fuel or Oxygen

Consider the problem of Section 7.1 under the assumption of complete stoichiometric combustion. As an example, assume again that the fuel is methane. Then the reaction is

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O \quad (69)$$

where excess fuel or excess oxygen brought into the reactor would lead to $\phi > 1$ or $\phi < 1$, and corresponding excess fuel or oxygen at the reactor output, respectively.

For k → CO_2 or H_2O and for excess oxygen to the reactor, i.e., for $\phi < 1$, the rate of generation of CO_2 and H_2O in the combustion is determined by the rate of supply of fuel to the reactor. Using Eqs. (9) and (69) it follows that

For the combustion of CH_4:

$$f_{CO2}^{(STOICH)}(\phi) \equiv \dot{\omega}_{CO2}/\dot{P}_{CH4,REACTIN} = 44/16 = 11/4 \text{ if } 0 < \phi \leq 1$$
$$f_{H2O}^{(STOICH)}(\phi) \equiv \dot{\omega}_{H2O}/\dot{P}_{FUEL,REACTIN} = 36/16 = 9/4 \text{ if } 0 < \phi \leq 1 \quad (70)$$

For k → CO_2 or H_2O and for excess fuel to the reactor, i.e., $\phi > 1$, the rate of generation of CO_2 and H_2O is determined by the rate of supply of oxygen to the reactor. It follows from Eq. (69) that

For complete stoichiometric combustion of CH_4:

$$\dot{\omega}_{CO2}/\dot{P}_{OXY,REACTIN} = 44/64 \text{ if } \phi \geq 1$$
$$\dot{\omega}_{H2O}/\dot{P}_{OXY,REACTIN} = 36/64 \text{ if } \phi \geq 1 \tag{71}$$

Using Eqs. (71) in Eq. (9) along with Eq. (36) and the definition of ϕ leads to

For complete stochiometric combustion of CH_4:

$$\begin{aligned} f_{CO2}^{(STOICH)}(\phi) &= (\dot{\omega}_{CO2}/\dot{P}_{CH4,REACTIN}) \\ &= (\dot{\omega}_{CO2}/\dot{P}_{OXY,REACTIN})/(r\phi) \\ &= (44/64)/[(16/64)\phi] = (11/4)/\phi \text{ if } \phi \geq 1 \\ f_{H2O}^{(STOICH)}(\phi) &= (\dot{\omega}_{H2O}/\dot{P}_{CH4,REACTIN}) \\ &= (\dot{\omega}_{H2O}/\dot{P}_{OXY,REACTIN})/[(\dot{P}_{CH4}/\dot{P}_{OXY})_{STOICH}\phi] \\ &= (36/64)/[(16/64)\phi] = (9/4)/\phi \text{ if } \phi \geq 1 \end{aligned} \tag{72}$$

It is noted that for the complete stoichiometric combustion of any fuel and for any k, the $f_k^{(STOICH)}(\phi)$ would have the identical form as that displayed above for methane, i.e.,

For complete stoichiometric combustion of any fuel and for any k:

$$f_k^{(STOICH)}(\phi) = C_k \text{ if } 0 < \phi \leq 1$$
$$f_k^{(STOICH)}(\phi) = C_k/\phi \text{ if } 1 < \phi \tag{73}$$

where the C_k are constants determined by the stoichiometric reaction. For k → fuel and oxygen, $C_{FUEL} = -1$ and $C_{OXY} = -1/(\dot{P}_{CH4}/\dot{P}_{OXY})_{STOICH}$, respectively, have already been presented in Eqs. (10) and (11).

7.2.2 Solutions for the $c_{k,U}$

Since complete stoichiometric combustion is assumed, Eqs. (19) and (20) can be used in Eq. (56), or Eqs. (10) and (11) in Eqs. (57) and (58). This leads to

If $0 \le \phi \le 1$:

$$m_U dc_{FUEL,U}/dt = -c_{FUEL,U}(\dot{m}_{FEEDBK} + \dot{m}_{FLOWIN}) \quad (74)$$

$$m_U dc_{OXY,U}/dt = -c_{OXY,U}(\phi\dot{m}_{FEEDBK} + \dot{m}_{FLOWIN}) + (1 - \phi)\dot{P}_{OXY,FLOWIN} \quad (75)$$

If $1 < \phi$:

$$m_U dc_{FUEL,U}/dt = -c_{FUEL,U}(\dot{m}_{FEEDBK}/\phi + \dot{m}_{FLOWIN}) + (1 - 1/\phi)\dot{P}_{FUEL,FLOWIN} \quad (76)$$

$$m_U dc_{OXY,U}/dt = -c_{OXY,U}(\dot{m}_{FEEDBK} + \dot{m}_{FLOWIN}) \quad (77)$$

where, again, $c_{FUEL,U}$ and $c_{OXY,U}$ would be subject to the initial conditions of Eqs. (62) and (63).

According to assumption b. above Eq. (50) the values $\dot{P}_{FUEL,FLOWIN}$ and $\dot{P}_{OXY,FLOWIN}$ are specified for a given experimental run. Also specified would be the value of r for the fuel being used, e.g., as with the value for methane given in Eq. (36). Then $\phi^{(SS)}$ can be calculated from Eq. (22). There are two possibilities, viz., $0 \le \phi^{(SS)} \le 1$ and $1 < \phi^{(SS)}$, and from Eqs. (42), (47), and (49) the value of $\dot{m}_{FEEDBK}$ for these are

$$\dot{m}_{FEEDBK} = \begin{cases} (c_{FUEL,U}/c_{FUEL,U}^{(MAX)})(1 - \phi^{(SS)})\dot{P}_{OXY,FLOWIN}/(c_{FUEL,U}^{(MAX)}r) \\ \qquad \text{if } 0 \le \phi^{(SS)} \le 1 \\ (c_{OXY,U}/c_{OXY,U}^{(MAX)})(1 - 1/\phi^{(SS)})\dot{P}_{FUEL,FLOWIN}/(c_{OXY,U}^{(MAX)}r) \\ \qquad \text{if } 1 < \phi^{(SS)} \end{cases} \quad (78)$$

Solutions for the two ranges of $\phi^{(SS)}$ will be obtained sequentially. Before discussing these, it is noted from Eqs. (22) and (59) and from the initial condition of Eq. (62) that $\phi(t = 0)$ will always satisfy

$$\phi(t = 0) \le \phi^{(SS)} \quad (79)$$

As t increases from zero, $\phi(t)$ will be expected to increase monotonically with t between $\phi(t = 0)$ and $\phi^{(SS)}$.

Case 1: $0 \le \phi^{(SS)} \le 1$

Here the top portion of Eq. (78) provides the required value for $\dot{m}_{FEEDBK}$. Using this in Eqs. (74) and (75) leads to

$$m_U dc_{FUEL,U}/dt = -c_{FUEL,U}\{(c_{FUEL,U}/c^{(MAX)}_{FUEL,U})(1 - \phi^{(SS)}) \cdot \dot{P}_{OXY,FLOWIN}/(c^{(MAX)}_{FUEL,U} r) + \dot{m}_{FLOWIN}\} \quad (80)$$

$$m_U dc_{OXY,U}/dt = -c_{OXY,U}\{(c_{FUEL,U}/c^{(MAX)}_{FUEL,U})\phi(1 - \phi^{(SS)}) \cdot \dot{P}_{OXY,FLOWIN}/(c^{(MAX)}_{FUEL,U} r) + \dot{m}_{FLOWIN}\} + (1 - \phi)\dot{P}_{OXY,FLOWIN} \quad (81)$$

Since $c_{FUEL,U}(t = 0) = 0$, it is evident from Eq. (80) that $dc_{FUEL,U}/dt$ is initially zero and will remain zero for all t. Therefore, for all t

$$c_{FUEL,U}(t) = 0 \quad (82)$$

In view of Eqs. (82) and (78), for the assumed complete stoichiometric reaction the model predicts $\dot{m}_{FEEDBK} = 0$ throughout an entire Case-1 experiment. Note that this is consistent with the discussion under the Case 1 of Section 5.4: $c_{OXY,U} \geq 0$, $c_{FUEL,U} = 0$. Also, it is clear from Eqs. (22) and (59) that the $\dot{m}_{FEEDBK} = 0$ result leads to the further conclusion that for all t

$$\phi(t) = \phi(t = 0) = \phi^{(SS)} \quad (83)$$

The results of Eqs. (73), (82), and(83) lead to significant simplification of Eqs. (65) and (80) which become

$$m_U dc_{OXY,U}/dt = -c_{OXY,U}\dot{m}_{FLOWIN} + (1 - \phi^{(SS)})\dot{P}_{OXY,FLOWIN} \quad (84)$$

$$m_U dc_{k,U}/dt + c_{k,U}\dot{m}_{FLOWIN} = \dot{P}_{FUEL,FLOWIN} C_k \quad \text{for k other than fuel or oxygen} \quad (85)$$

where, as determined in Eqs. (71) and (72), $C_{CO2} = 11/4$ and $C_{H2O} = 9/4$ when the fuel is CH_4.

It is convenient to define the dimensionless variables τ, ψ_{OXY}, ψ_k, and μ, and the dimensionless parameter β:

$$\tau = t\dot{m}_{FLOWIN}/m_U(t=0) = t\dot{m}_{FLOWIN}RT_U(t=0)/(Vp_{AMB}) = t/t^* \quad (86)$$

$$\psi_{OXY} = c_{OXY,U}(t)/c_{OXY,U}(t=0) = c_{OXY,U}(t)/c_{OXY,U}^{(MAX)} \quad (87)$$

$$\psi_k = c_{k,U}(t)\dot{m}_{FLOWIN}/[\dot{P}_{FUEL,FLOWIN}f_k(\phi^{(SS)})] \quad \text{for k other than fuel or oxygen} \quad (88)$$

$$\mu = \mu(\tau) = m_U(t)/m_U(t=0) = T_U(t=0)/T_U(t) = T_U(t=0)/T_U(t^*\tau) \quad (89)$$

$$\beta = [(\phi^{(SS)} - 1)\dot{P}_{OXY,FLOWIN}/\dot{m}_{FLOWIN}]/c_{OXY,U}^{(MAX)}$$

$$= (1 - 1/\phi^{(SS)})/(c_{OXY,U}^{(MAX)}r + 1/\phi^{(SS)}) \quad (90)$$

where

$$t^* = Vp_{AMB}/[\dot{m}_{FLOWIN}RT_U(t=0)] \quad (91)$$

According to Eq. (29), for the present range of $\phi^{(SS)}$

$$\beta = -c_{OXY,REACTOUT,STOICH}^{(SS)}/c_{OXY,U}^{(MAX)} \quad \text{if } 0 \le \phi^{(SS)} \le 1 \quad (92)$$

Note that here β must satisfy

$$-1 \le \beta \le 0 \quad (93)$$

where $\beta \to -1$ corresponds to $\phi^{(SS)} \to 0$ (when $\dot{P}_{FUEL,FLOWIN}$ becomes negligible and $\dot{P}_{OXY,FLOWIN}/\dot{m}_{FLOWIN} \to c_{OXY,U}^{(MAX)} = 0.232$) and $\beta = 0$ corresponds to $\phi^{(SS)} = 1$, the upper limit for $\phi^{(SS)}$ in the present case.

Using Eqs. (86)-(90) in Eqs. (81) and (63) and in Eqs. (65) and (68), and making the final transformation

$$\sigma = \int_0^\tau d\eta/\mu(\eta) \quad (93)$$

leads to

$$d\psi_{OXY}/d\sigma = -\psi_{OXY} - \beta; \quad \psi_{OXY}(0) = 1 \quad (94)$$

$$d\psi_k/d\sigma = -\psi_k + 1; \quad \psi_k(0) = 0 \quad \text{for k other than fuel or oxygen} \quad (95)$$

The solutions to Eqs. (94) and (95) are

$$(\psi_{OXY} + \beta)/(1 + \beta) = \exp(-\sigma) \tag{96}$$

$$\psi_k = 1 - \exp(-\sigma) \quad \text{for k other than fuel and oxygen} \tag{97}$$

The solution concentrations $c_{OXY,U}(t)$ and $c_{k,U}(t)$ of Eqs. (96) and (97) exhibit the expected transition from their initial to their steady state values, the latter corresponding to $\lim \sigma \to \infty$ $(\psi_{OXY}, \psi_t) = (-\beta, 0)$. Here the transition process involves simple dilution of the upper layer by the steady and constant stream (i.e., corresponding to $\phi = \phi^{(SS)} = \text{constant}$) flowing from the reactor. Plots of these results will be presented below.

Case 2: $1 < \phi^{(SS)}$

Here the bottom portion of Eq. (78) provides the required value for $\dot{m}_{FEEDBK}$, which is no longer zero. Using this in Eq. (59) along with the initial conditions of Eqs. (62) and (63), it can be shown that for all possible experimental runs covered by the present Case 2, the model predicts $\phi(t = 0) = 1$. Accordingly, for this case, from Eqs. (74)-(77), only Eqs. (76) and (77) need to be considered.

The dimensionless variable ψ_{FUEL} is defined as

$$\psi_{FUEL} = c_{FUEL,U}/c^{(SS)}_{FUEL,REACTOUT,STOICH} \tag{98}$$

Also, according to Eq. (28), for the present range of $\phi^{(SS)}$

$$\beta = c^{(SS)}_{FUEL,REACTOUT,STOICH}/(c^{(MAX)}_{OXY,U} r) \text{ if } 1 < \phi^{(SS)} \tag{99}$$

Note that here β must satisfy

$$0 < \beta \leq 1/(c^{(MAX)}_{OXY,U}) \text{ if } 1 < \phi^{(SS)} \tag{100}$$

where according to Eq. (90), $\beta \to 1/[c^{(MAX)}_{OXY,U}(\dot{P}_{FUEL}/\dot{P}_{OXY})_{STOICH}]$ corresponds to $\phi^{(SS)} \to \infty$, i.e., an experiment with the fuel source embedded in the upper layer and with no oxygen supply ($\dot{P}_{OXY,FLOWIN} = 0$), and $\beta \to 0$ corresponds to $\phi(t = 0) = \phi^{(SS)} \to 1$. For CH_4, the upper limit for $\beta \approx 1/[0.232(1/4)] \approx 17.24$.

Using Eqs. (22), (73), and (78) and the above definitions for ψ_{FUEL}, ψ_{OXY}, and β in Eqs. (59), (66), (76), and (77) leads to

If $1 < \phi = \phi^{(SS)}[1 + \beta(1 - 1/\phi^{(SS)})\psi_{FUEL}\psi_{OXY}]/[1 + (\phi^{(SS)} - 1)\psi_{OXY}^2]$:

(101)

$$d\psi_{FUEL}/d\sigma = -(\beta\psi_{OXY} + 1)\psi_{FUEL} + [1 + \beta\psi_{OXY}\psi_{FUEL} - \psi_{OXY}^2]/[1 + \beta(1 - 1/\phi^{(SS)})\psi_{OXY}\psi_{FUEL}] \quad (102)$$

$$d\psi_{OXY}/d\sigma = -(\beta\psi_{OXY} + 1)\psi_{OXY} \quad (103)$$

$$d\psi_k/d\sigma + \psi_k = [\psi_{OXY}^2(1 - 1/\phi^{(SS)}) + 1/\phi^{(SS)}] \quad \text{for k other than fuel and oxygen} \quad (104)$$

$$\psi_{OXY}(0) = 1 \quad (105)$$

$$\psi_{FUEL}(0) = 0 \quad (106)$$

$$\psi_k(0) = 0 \quad \text{for k other than fuel and oxygen} \quad (107)$$

Note that in obtaining Eq. (104), the second of Eqs. (73) was used to show that for complete stoichiometric combustion and for any $\phi > 1$, as in the present case,

$$\phi f_k(\phi)/[\phi^{(SS)} f_k(\phi^{(SS)})] = 1 \text{ for all k} \quad (108)$$

The solution of Eqs. (103) and (105) for ψ_{OXY} is found to be

$$\psi_{OXY} = \exp(-\sigma)/\{1 + \beta[1 - \exp(-\sigma)]\} \quad (109)$$

and this is plotted in Figure 11 with parameter β in the range $0 < \beta \leq 20$. Using Eq. (110), the solution of Eqs. (105) and (108) for ψ_k is found to be

$$\psi_k = [1 - \exp(-\sigma)][1/\phi^{(SS)} + (1 - 1/\phi^{(SS)})\psi_{OXY}] \quad (110)$$

Eq. (109) has been used to carry out numerical integrations of Eqs. (102) and (106) for ψ_{FUEL}.

7.2.3. Plotting of the Solutions

The solutions for ψ_{OXY}, ψ_{FUEL}, and ψ_k are plotted in Figures 9 and 10 for the entire range of β and $\phi^{(SS)}$, respectively. To prepare these plots it was convenient to use the result

$$\phi^{(SS)} = (1 + \beta)/(1 - \beta c_{OXY,U}^{(MAX)} r) \qquad (111)$$

which was obtained from Eq. (90).

The Figure 9 plots present the dimensionless concentrations as a function of dimensionless time with β as a parameter.

Consistent with the Case-1 results of Eqs. (96) and (97), in the entire range $-1 \leq \beta \leq 0$ ψ_k is seen in Figure (9) to be independent of both β and fuel-type, i.e., r, while ψ_{OXY} depends on β, but is otherwise independent of fuel-type. Also, for this β range and for the corresponding $\phi^{(SS)}$ range $0 \leq \phi^{(SS)} \leq 1$, oxygen concentration is identically zero according to Eq. (82) and no dimensionless variable for this concentration was required in the analysis.

Consistent with the Case-2 results of Eqs. (102), (106), (109), and (110) and by the definition of Eq. (90), for $\beta > 0$ all dimensionless concentrations depend on both β and fuel-type. In this range of β, the actual results plotted in Figure 9 are those that correspond to the use of CH_4 as the fuel, i.e., r taken to be 1/4.

Recall that $\beta > 0$ is a necessary condition for the steady state value of $c_{FUEL,U}$ to be non-zero, and that ψ_{FUEL} was defined only in this β range as the concentration $C_{FUEL,U}$ made dimensionless by normalizing with its steady state value. Thus, as indicated in the plots, ψ_{FUEL} solutions only exist for $\beta > 0$. It is noteworthy that for CH_4, ψ_{FUEL} is relatively insensitive to variations in β in the entire applicable range of β.

All results are also presented in Figure 10, where plots of the ψ's are given as functions of σ with $\phi^{(SS)}$ as a parameter. Such plots depend on fuel-type for the entire range of $\phi^{(SS)}$. The actual plots presented correspond again to use of CH_4 as the fuel.

Figure 11 highlights the ψ solutions when $\phi^{(SS)} \to \infty$ and when CH_4 is the fuel, i.e., when $\beta \approx 17.23$. As mentioned earlier, this corresponds to experimental runs where the fuel is methane and where the fuel source is submerged in the upper layer with no source of oxygen. As has been observed in reference [9], such configurations lead to extinguishment of the flame at the time when $C_{OXY,U}$ drops to approximately 0.15, i.e., when ψ_{OXY} drops to 0.15/0.23 = 0.65. As can be seen in the figure, this occurs when σ is approximately σ_{EXT} = 0.030. Thus, using the complete stoichiometric combustion approximation, the present model predicts that a methane flame will extinguish in a Figure 4b experimental configuration at the time, t_{EXT}, when

$$\int_0^{t_{EXT}} [T(t)/T(t=0)]dt = t^* \sigma_{EXT} = 0.030 V p_{AMB}/[\dot{m}_{FLOWIN} R T_U(t=0)] \qquad (112)$$

8. Summary and Conclusions

A general model was developed for predicting the generation rates of oxygen, fuel, and any other products of combustion of interest in rooms containing a fire. The model is called the generalized global equivalence ratio model. It extends the steady state global equivalence ratio model established previously in the steady-state experimental studies of references [3]-[7].

In Section 6, a concise algorithm was presented for implementing the model in two-layer zone-type fire models. This would be used in simulating the distribution of products of combustion in multi-room fire environments.

Section 7 was devoted to an example application of the model. There, the model was used to formulate the general initial-value problems for the transient concentrations of all products of combustion in some of the above-mentioned experimental studies. The problems were solved under the constraint that only complete stoichiometric combustion processes are involved. Solutions for the concentrations were obtained and presented for arbitrary experimental conditions. As a final result, the solutions were used to predict the time-to-extinguishment of a burning fuel source embedded in an initially ambient-atmosphere upper layer.

The results of this work suggest that a follow-up effort be carried out involving the following activities:

a. The algorithm of the generalized global equivalence ratio model should be coded and documented as a modular subroutine for general use in an arbitrary two-layer zone-type fire model.

b. The subroutine of Item a. should be tested by using it to obtain Section 7-type solutions for transient concentrations, but with the complete stoichiometric combustion constraint removed.

c. The solutions of Item b. and those of the present work should be compared with time-dependent data acquired from new or re-run reference [3], [4], and/or [7]-type experiments.

d. The subroutine of Item a. should be implemented and tested in an existing multi-room zone-type fire model; simulated results should be compared to data acquired in full-scale room fire experiments.

e. Research on the effect of temperature on global equivalence ratio-type correlations should be continued, and based on the results of this, the model presented here should be modified appropriately.

f. Ignition criteria for initiation of relatively fuel-rich layer burning and appropriate modification of the combustion model under layer burning conditions should be developed and taken account of in a revised version of the present model. It would appear that the ignition criteria could be based on a extension to the ideas developed in reference [8].

g. Develop a test method for determining the $f_k(\phi)$ for different combustibles of interest and establish the validity of the model for practical combustibles.

h. Investigate valid means of extending the model to practical combustibles involving multiple fuels.

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NOMENCLATURE

$c_{FUEL,U}^{(MAX)}$	maximum possible value of $c_{FUEL,U}$, taken to be 1
$c_{k,L}$ [$c_{k,U}$]	mass fraction of combustion product k in the lower [upper] layer
$c_{k,REACTOUT}$	mass fraction of combustion product k in the reactor outflow
$c_{k,REACTOUT,STOICH}$	value of $c_{k,REACTOUT}$ for stoichiometric combustion
$c_{k,REACTOUT}^{(SS)}$	value of $c_{k,REACTOUT}$ under steady state conditions
$c_{k,U}^{(SS)}$	value of $c_{k,U}$ under steady state conditions
$c_{k,REACTOUT}^{(SS,FIT)}(\phi)$	correlation functions fitted to experimentally determined product k mass fraction data
$c_{OXY,U}^{(MAX)}$	maximum possible value of $c_{OXY,U}$, taken to be 0.232
$f_k(\phi)$	Eq. (9)
$f_k^{(STOICH)}$	value of $f_k(\phi)$ for stoichiometric combustion
m_L [m_U]	total mass in the lower [upper] layer
$\dot{m}_{FEEDBK}$	mass flow rate to the reactor from the bulk of the upper layer
$\dot{m}_{FEEDBK,1}$	value of $\dot{m}_{FEEDBK}$ under Case 1 conditions, Eq. (40)
$\dot{m}_{FEEDBK,2}$	value of $\dot{m}_{FEEDBK}$ under Case 2 conditions, Eq. (48)
$\dot{m}_{FEEDBK,3}$	value of $\dot{m}_{FEEDBK}$ under Case 3 conditions, Eq. (44)
$\dot{m}_{FEEDBK}^{(1)}$	characteristic value of $\dot{m}_{FEEDBK,1}$
$\dot{m}_{FEEDBK}^{(3)}$	characteristic value of $\dot{m}_{FEEDBK,3}$
$\dot{m}_{FLOWIN}$ [$\dot{m}_{FLOWOUT}$]	total mass flow rate into [out of] the upper layer
$(\dot{P}_{FUEL}/\dot{P}_{OXY})_{STOICH}$	stoichiometric fuel-to-oxygen ratio
$\dot{P}_{k,FEEDBK}$	mass flow rate of combustion product k into the reactor from the bulk of the upper layer
$\dot{P}_{k,FLOWIN}$ [$\dot{P}_{k,FLOWOUT}$]	sum of rates of flow of all components of product k into [out of] the upper layer
$P_{k,L}$ [$P_{k,U}$]	mass of combustion product k in the lower [upper] layer

$\dot{P}_{k,L}$ $[\dot{P}_{k,U}]$	net rates of combustion product k flowing to the lower [upper] layer
$\dot{P}_{k,REACTIN}$	net mass flow rate of combustion product k into the reactor
$\dot{P}_{k,REACTOUT}$	net mass flow rate of combustion product k out of the reactor
R	ideal gas constant for air
r	$(\dot{P}_{FUEL}/\dot{P}_{OXY})_{STOICH}$
T_{AMB}	temperature of the laboratory
T_U	temperature of the upper layer
t	time
t^*	characteristic value of t (91)
t_{EXT}	value of t at extinction of CU_4 flame
V	volume of the collector
α_{FUEL}, α_{OXY}	coefficients in $\dot{m}_{FEEDBK}$ equation
β	dimensionless parameter
μ	dimensionless value of m_U
ρ_U	density of the upper layer
σ	transformed value of τ
τ	dimensionless value of t
ϕ	Eq. (7)
$\phi^{(SS)}$	value of ϕ under steady state conditions
ϕ_{FUEL}	Eq. (26)
ϕ_{OXY}	Eq. (27)
σ_{EXT}	value of σ at extinction of CH_4 flame
ψ_k, ψ_{FUEL}, ψ_{OXY}	dimensionless values of $c_{k,U}$, $c_{FUEL,U}$, $c_{OXY,U}$
$\dot{\omega}_k$	mass generation rate of combustion product k

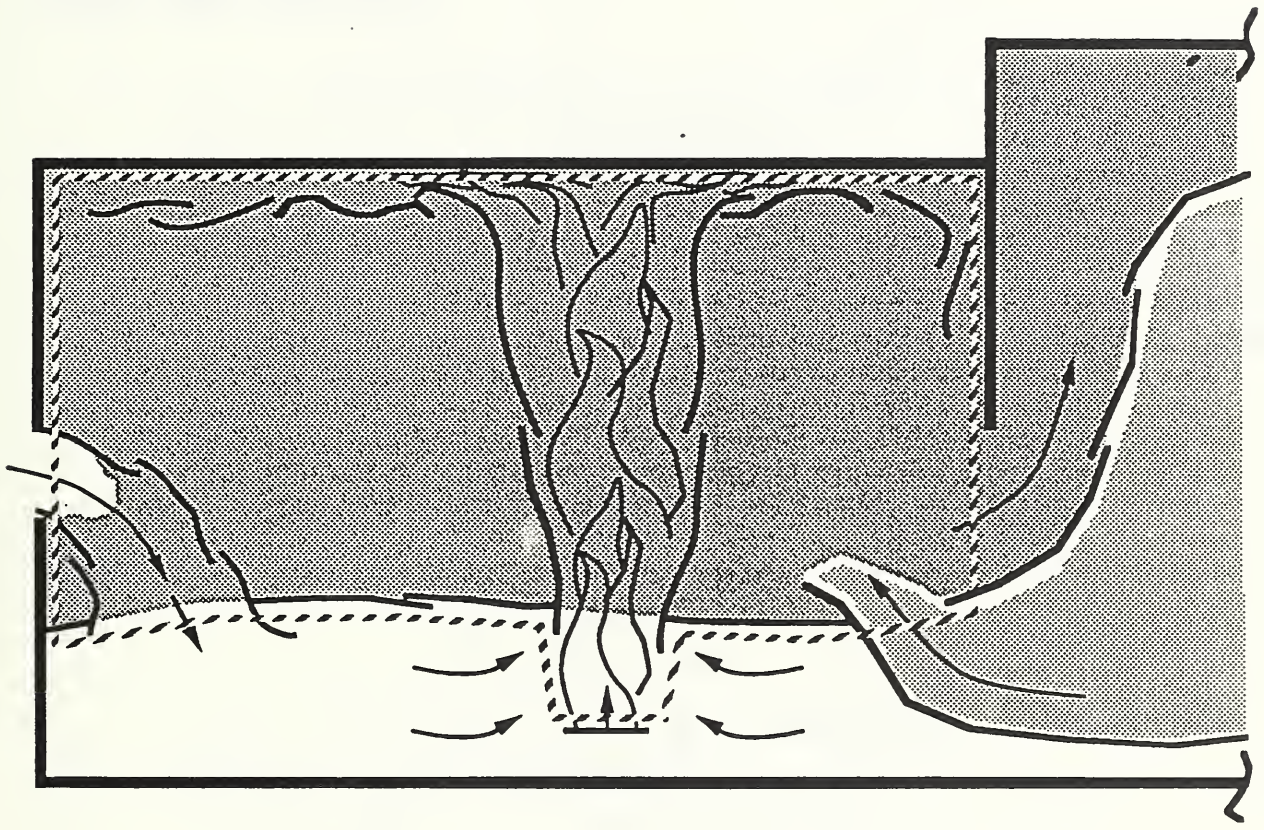

Figure 1. The extended upper layer in a room of fire origin which includes the assumed negligible-volume fire plume.

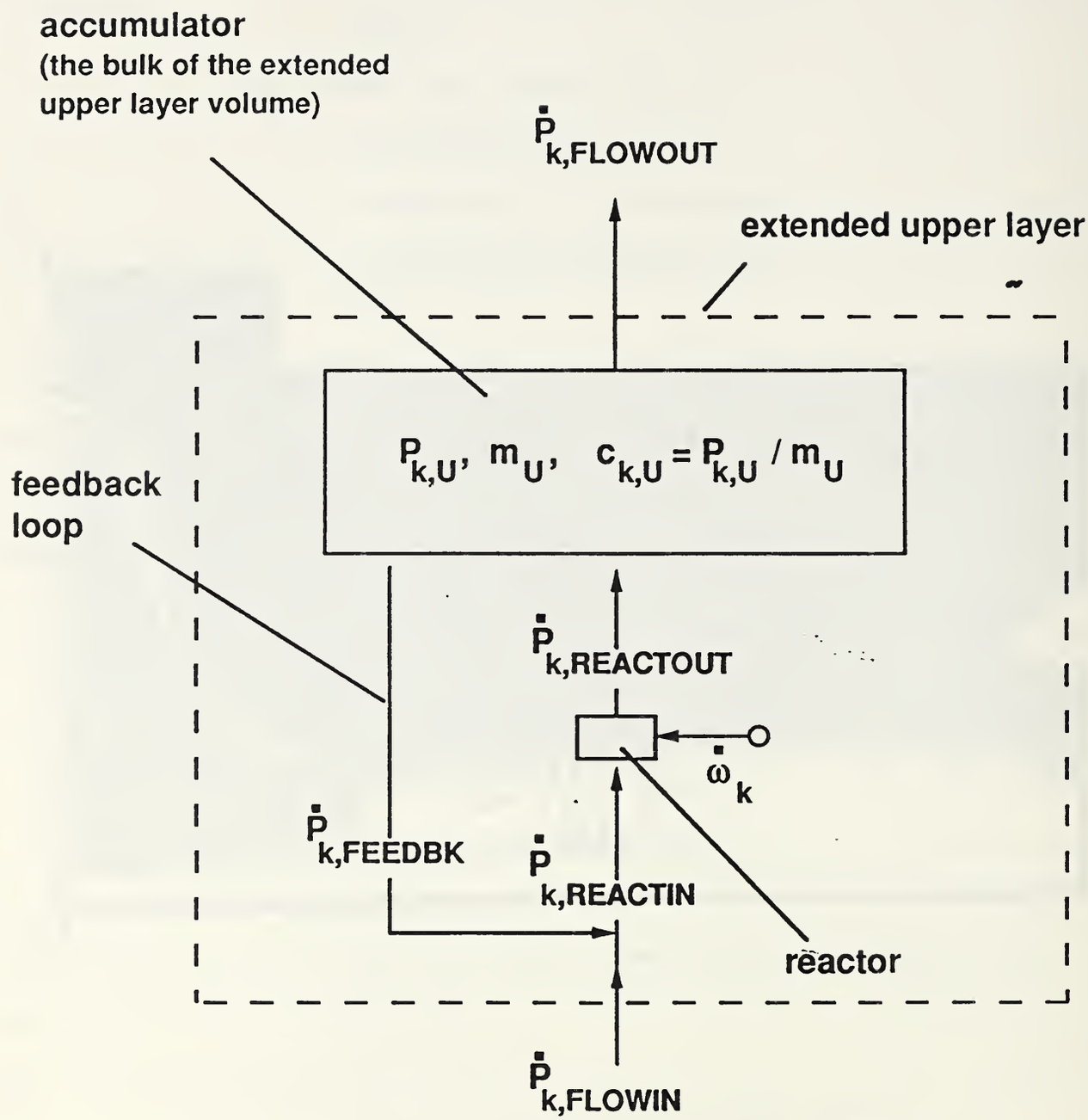

Figure 2. The model of combustion and flow dynamics in the extended upper-layer of Figure 1.

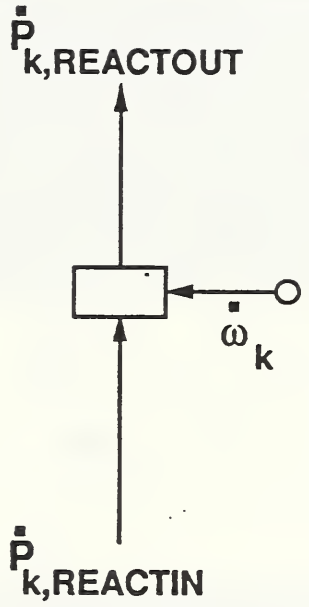

Figure 3. An isolated view of the reactor of Figure 2.

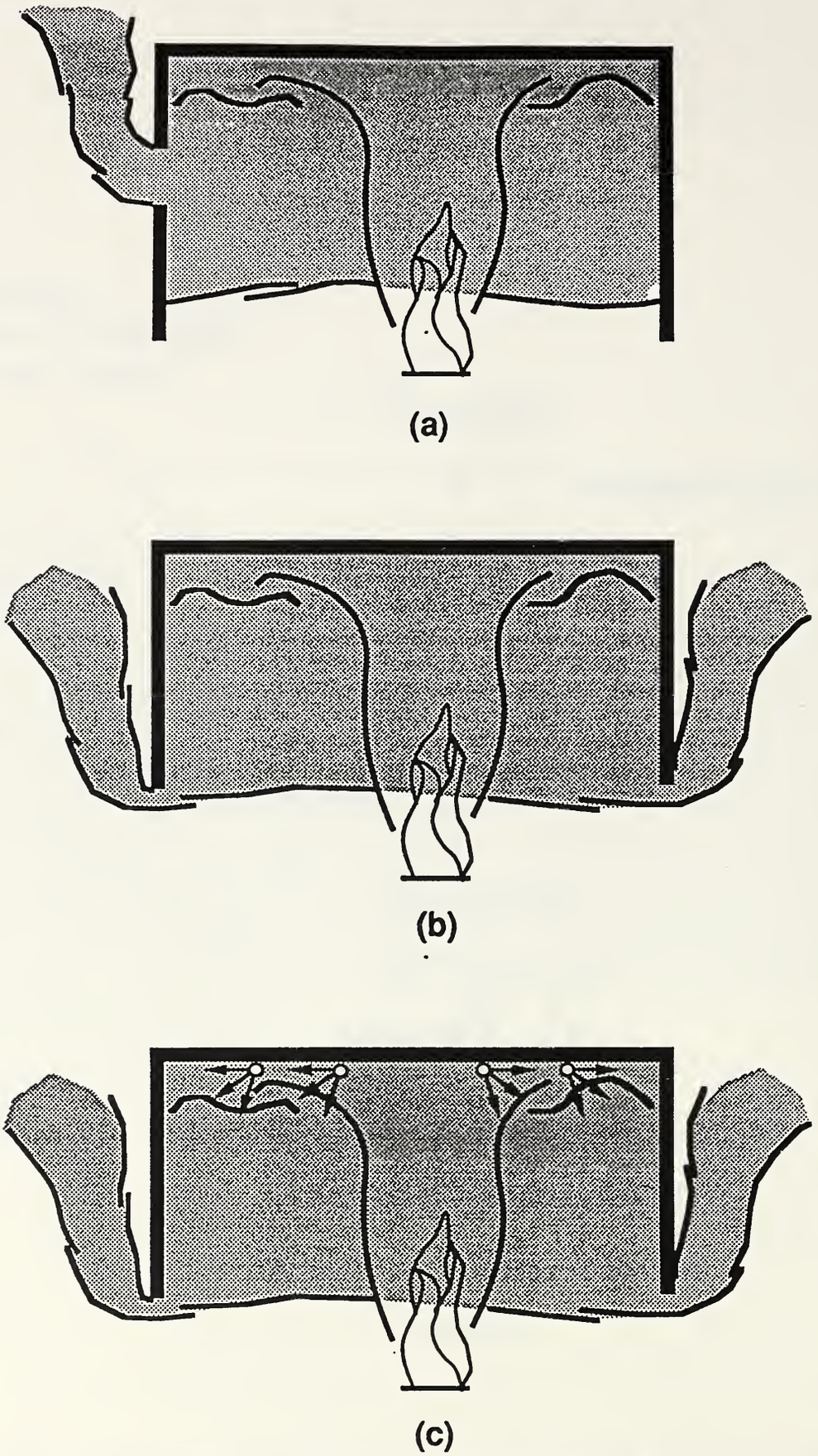

Figure 4. The experimental configuration used in [5] and [6] (a), in [4] (b), and in [3] and [7] (c).

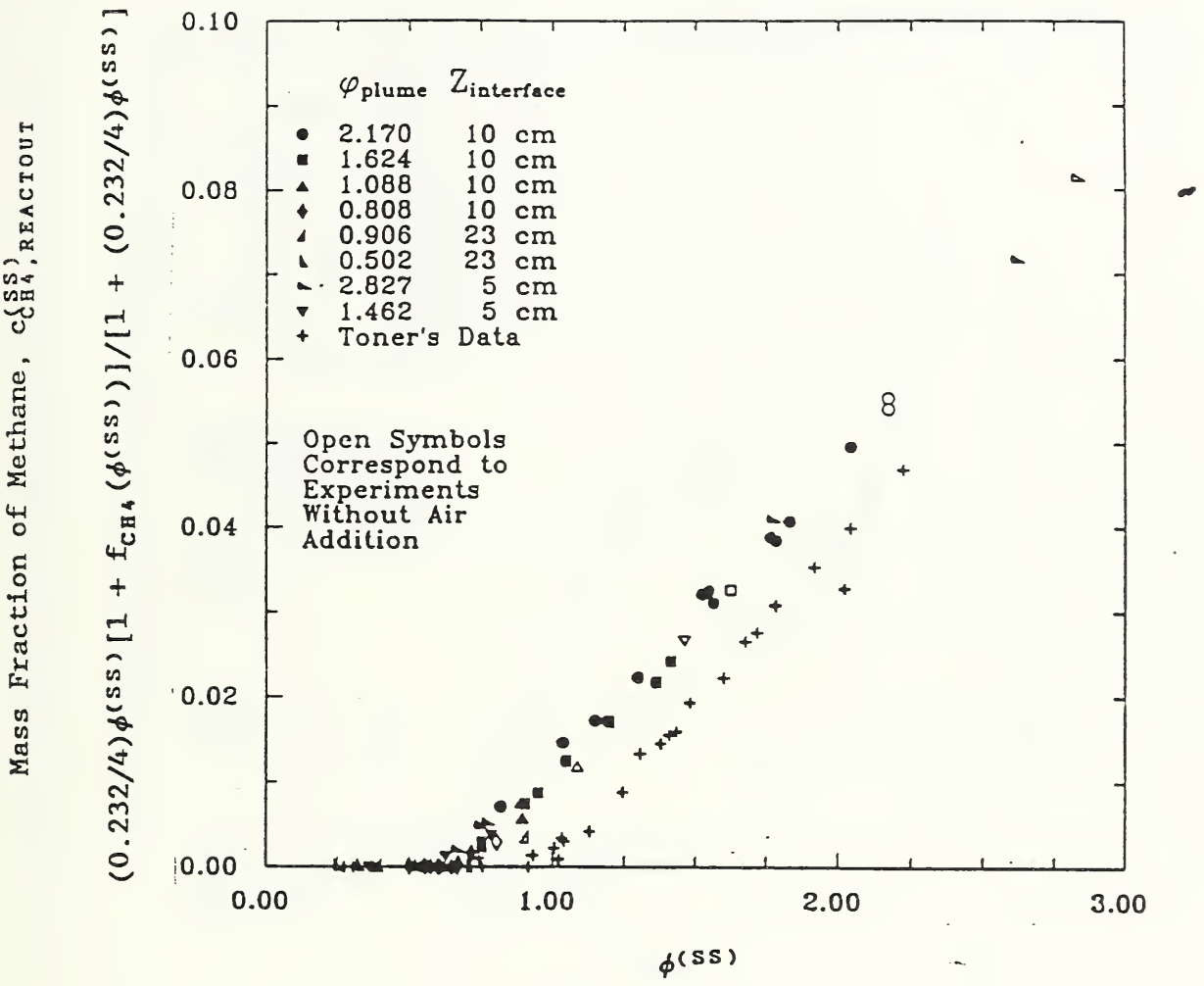

Figure 5. Relabeled Figure 3 of [7] according to Eq. (37) for data of $c^{(SS)}_{CH4,REACTOUT}$.

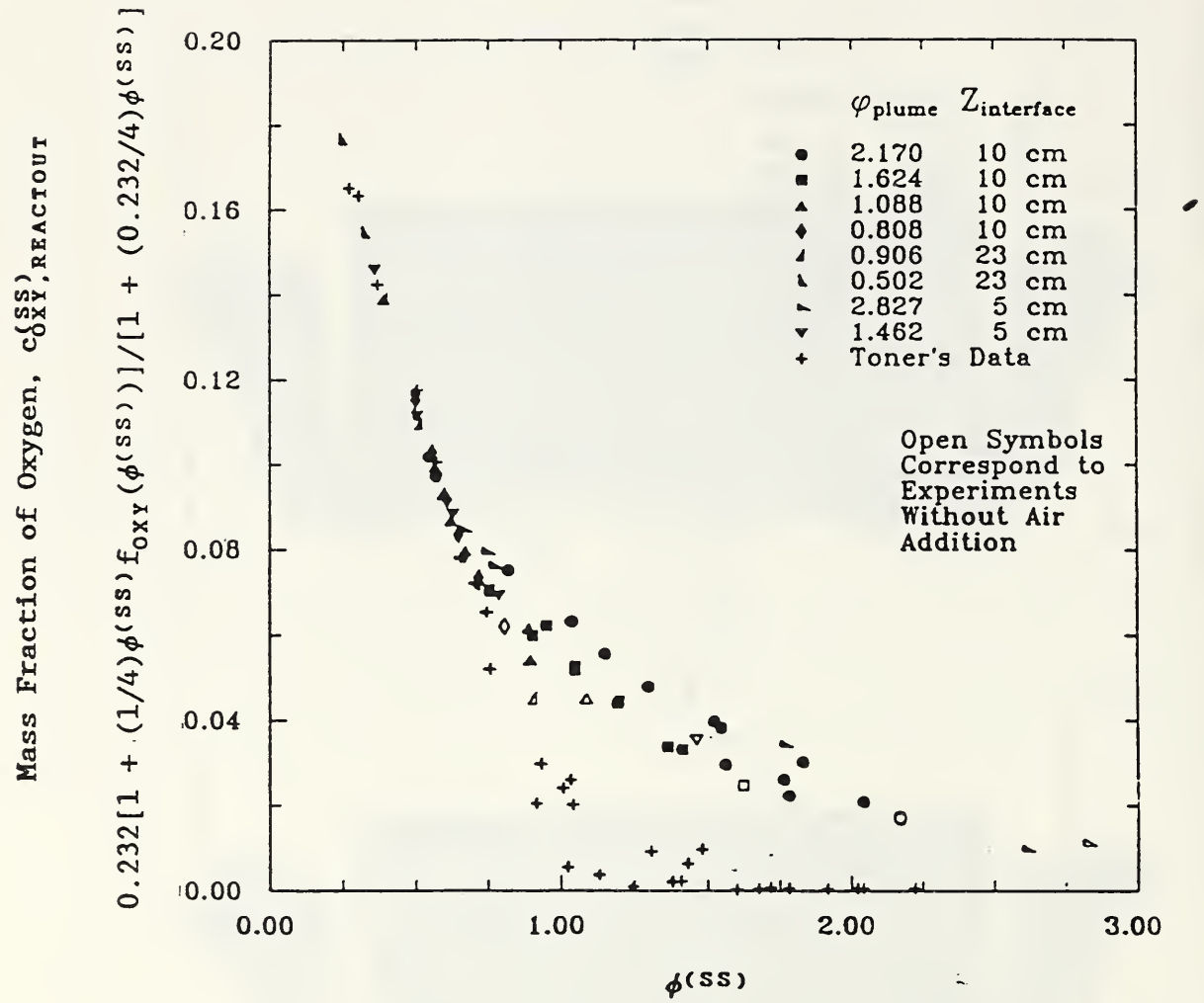

Figure 6. Relabeled Figure 1 of [7] according to Eq. (38) for data of $c^{(SS)}_{OXY,REACTOUT}$.

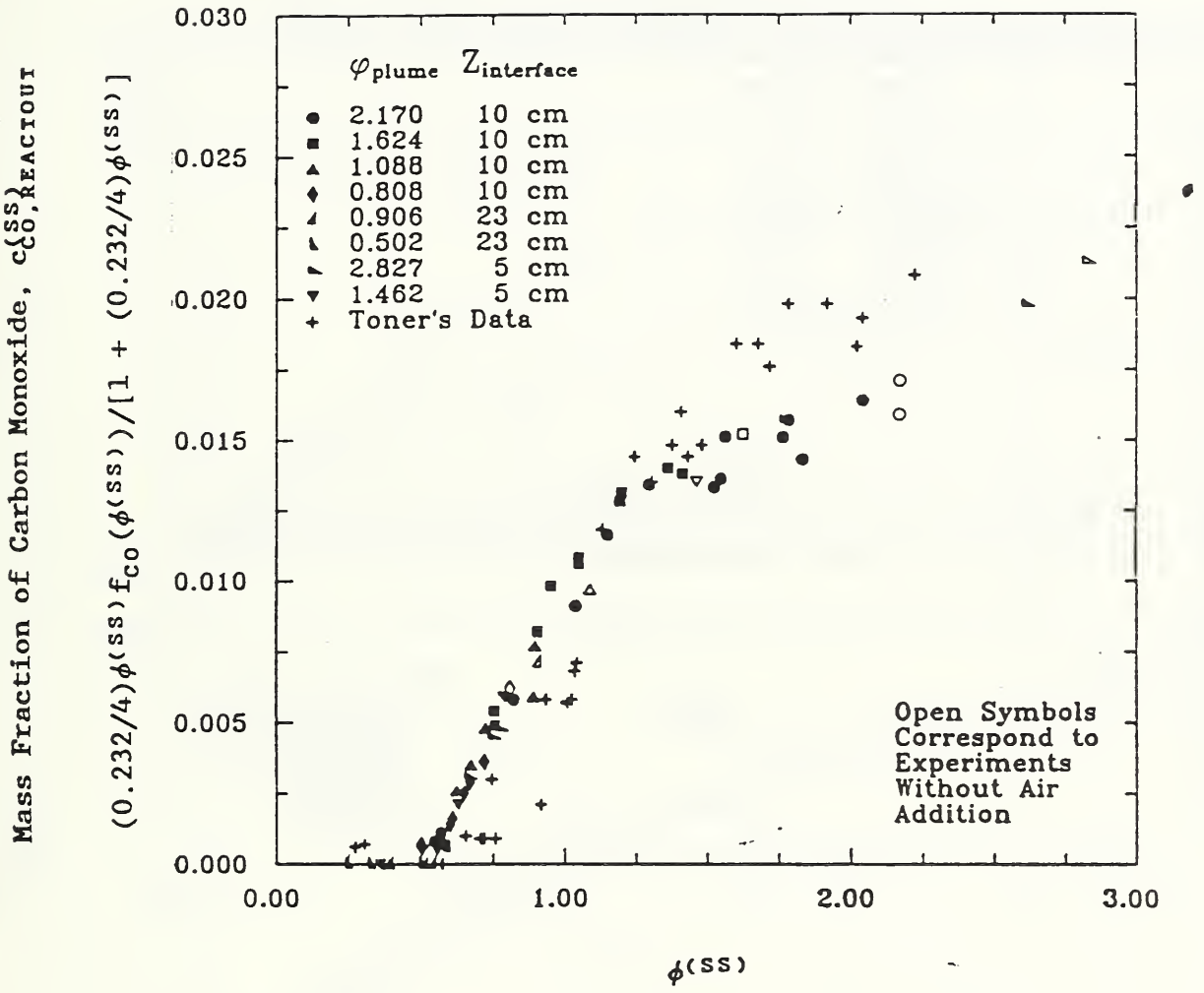

Figure 7. Relabeled Figure 2 of [7] according to Eq. (39) for data of $c_{CO,REACTOUT}^{(SS)}$.

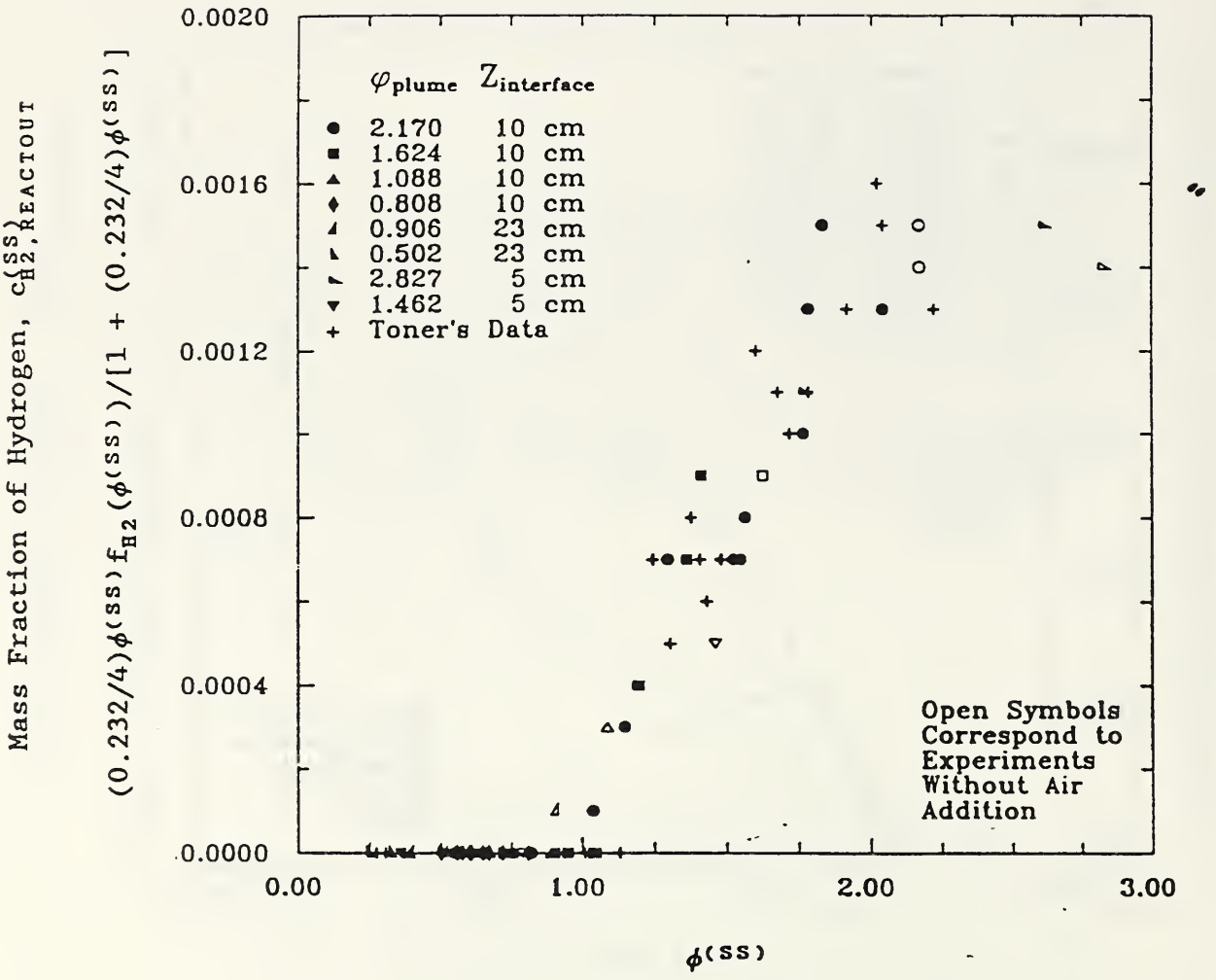

Figure 8. Relabeled Figure 4 of [7] according to Eq. (39) for data of $c^{(SS)}_{H2,REACTOUT}$.

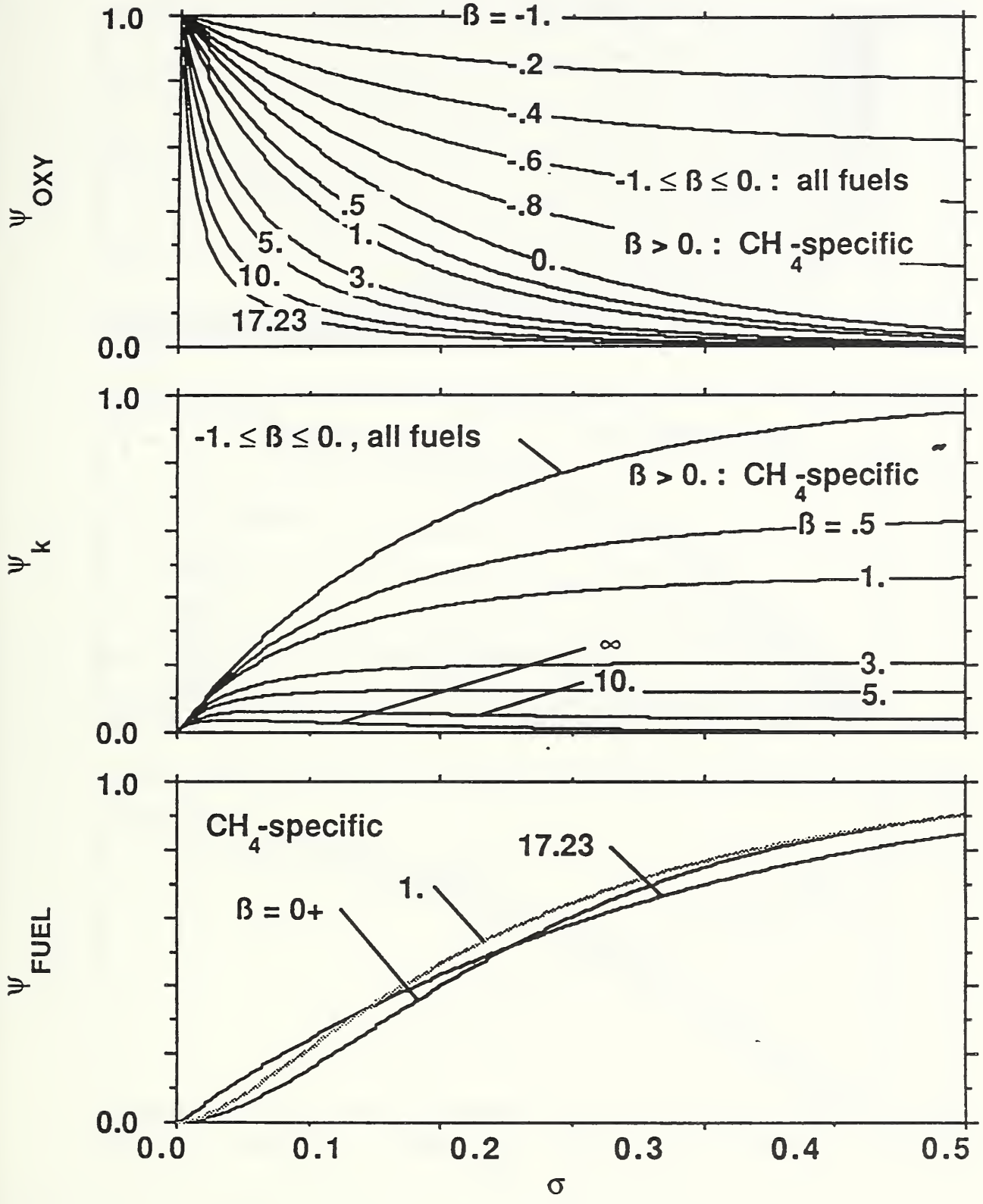

Figure 9. Plots of dimensionless concentrations ψ_{OXY}, ψ_k, and ψ_{FUEL} as a functions of dimensionless time, σ, with β as a parameter, where the results, are fuel-independent for $-1 \leq \beta \leq 0$, and CH_4-specific for $\beta > 1$.

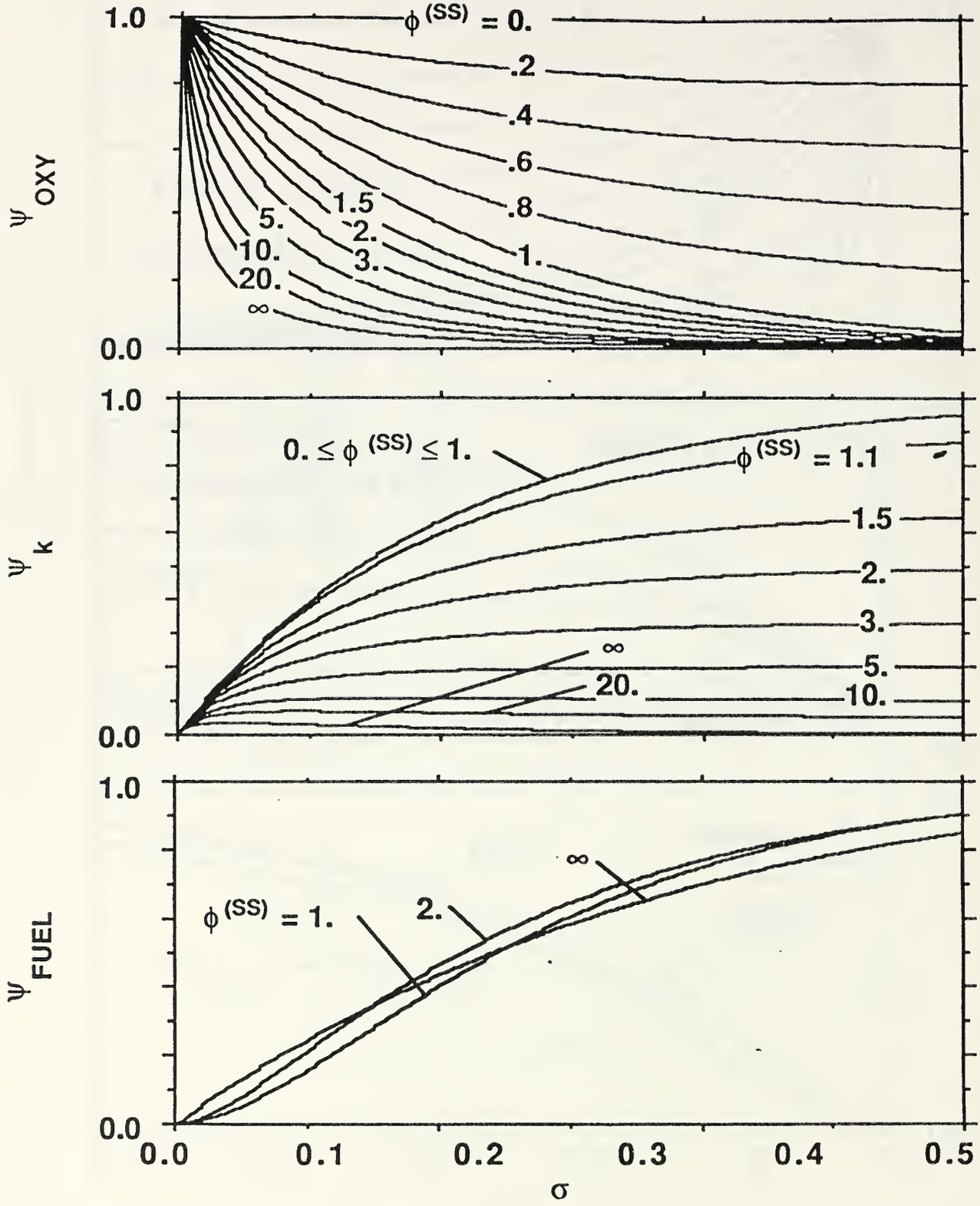

Figure 10. Plots of dimensionless concentrations ψ_{OXY}, ψ_k, and ψ_{FUEL} as a functions of dimensionless time, σ, with $\phi^{(SS)}$ as a parameter when CH_4 is the fuel, i.e., when $(\dot{P}_{FUEL}/\dot{P}_{OXY})_{STOICH} = 1/4$.

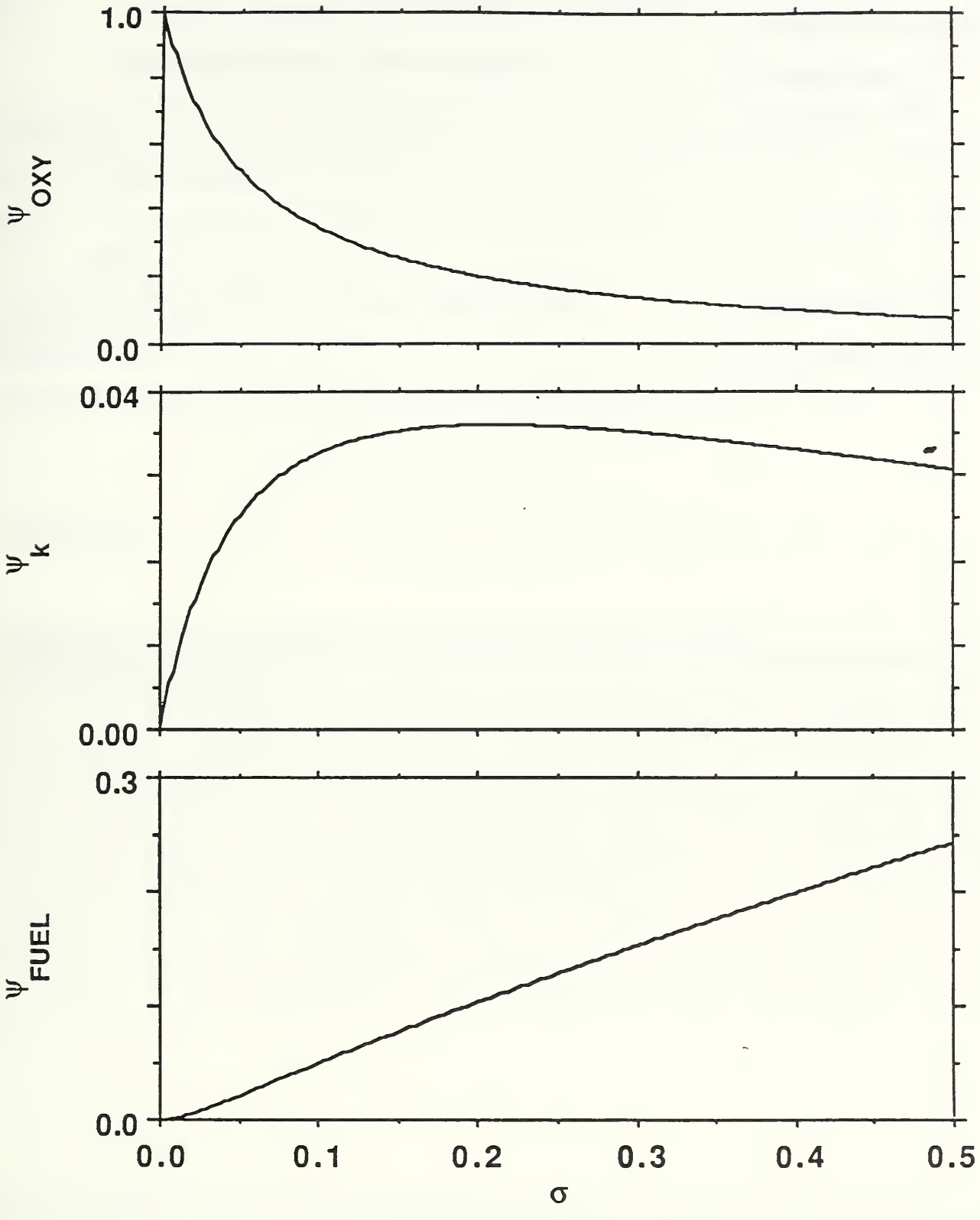

Figure 11. Plots of dimensionless concentrations ψ_{OXY}, ψ_k, and ψ_{FUEL} as a functions of dimensionless time, σ, when $\phi^{(SS)} \to \infty$ and when CH_4 is the fuel, i.e., $\beta \approx 17.23$

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11. ABSTRACT (A 200-WORD OR LESS FACTUAL SUMMARY OF MOST SIGNIFICANT INFORMATION. IF DOCUMENT INCLUDES A SIGNIFICANT BIBLIOGRAPHY OR LITERATURE SURVEY, MENTION IT HERE.)

A general model is developed for predicting the generation rates of oxygen, fuel, and any other products of combustion of interest in rooms containing fires. The model is called the generalized global equivalence ratio model. It extends the steady state global equivalence ratio model established from steady-state data of several previous experimental studies. After presenting the details, a concise algorithm is outlined for implementing the model in two-layer zone-type compartment fire model computer codes. With the algorithm in place, such codes could be used to simulate the distribution of proeducts of combustion in single or multi-room fire environments. In an example application, the model is used to simulate the time-dependent environment, including that of steady-state, in some of the above-mentioned experimental studies. For arbitrary experimental conditions and under the assumption of stoichiometric combustion, solutions for concentrations of products of combustion are obtained and presented. In one concise result, the solutions are used to predict the time-to- extinguishment of a burning methane fuel source embedded in an initially ambient-atmosphere upper layer.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)
building fires; combustion; compartment fires; computer models; fire models; mathematical models; zone models

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